Virtual Process Engineering

in coarse-grained discrete particle methods

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2017.08.08

What is virtual process engineering

Virtual experiment and measurement on digital processes in computers

High fidelity: Indistinguishable to the real processes
Realtime/quasi-realtime

High flexibility: Virtual and real systems integrated:
experiment-measurement-computation
-visualization-control integrated

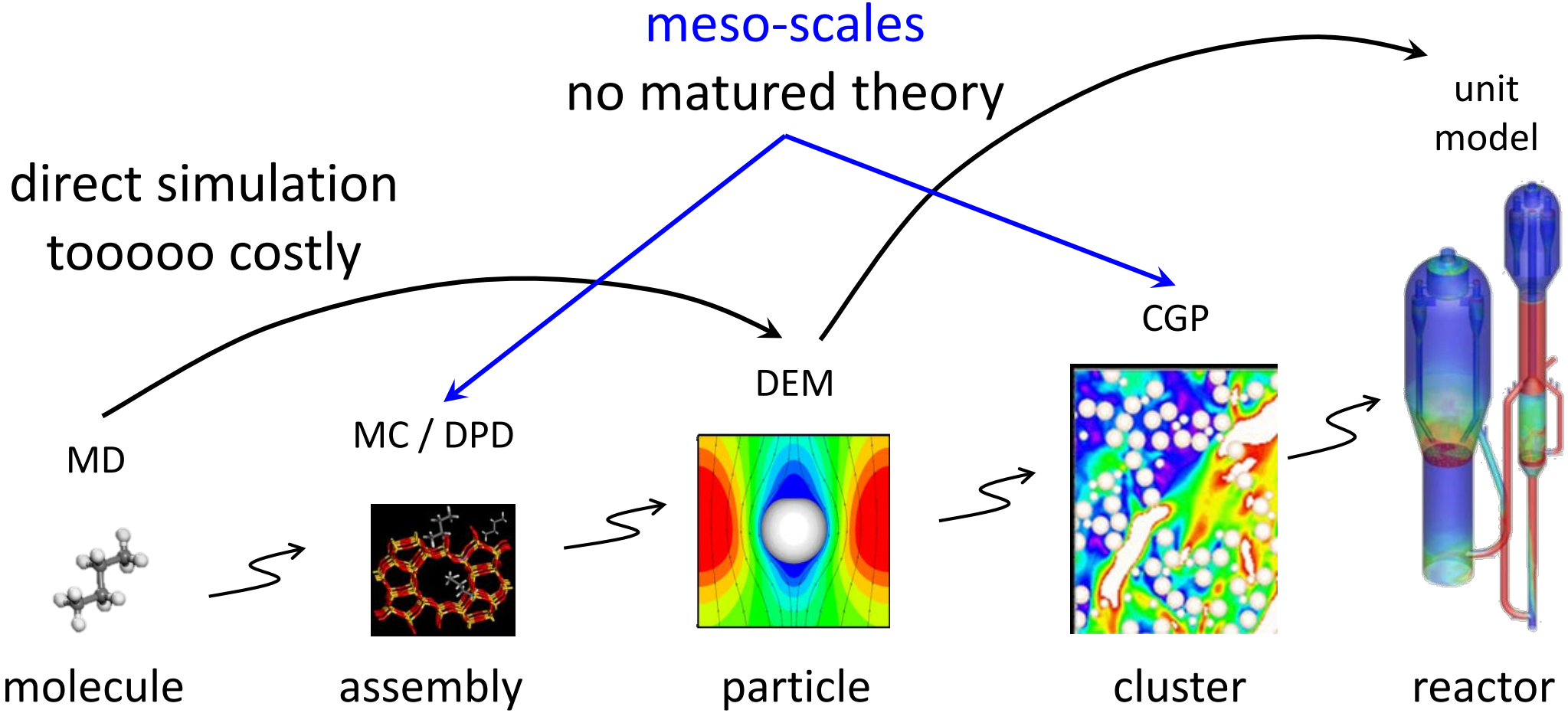
High efficiency: Within reasonable cost and complexity

New R&D and training/educational platform

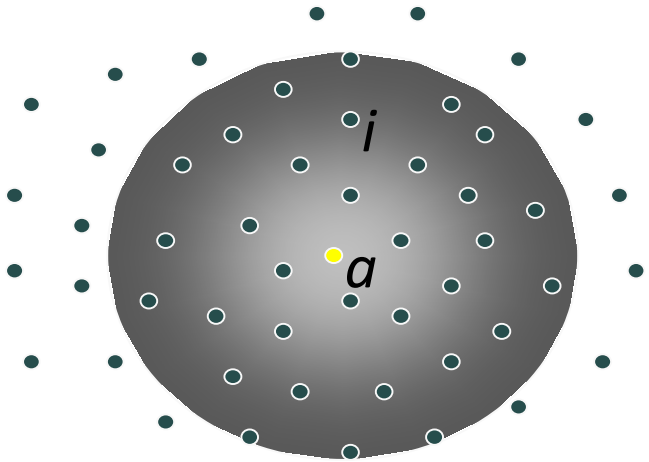
Ge et al. 2011 *Chem. Eng. Sci.* 66:4426-4458; Liu et al. 2012 *Chem. Eng. Proc.* 108:28-33

Why
discrete particle methods

Challenges of multi-scale simulation



Advantages of discrete methods

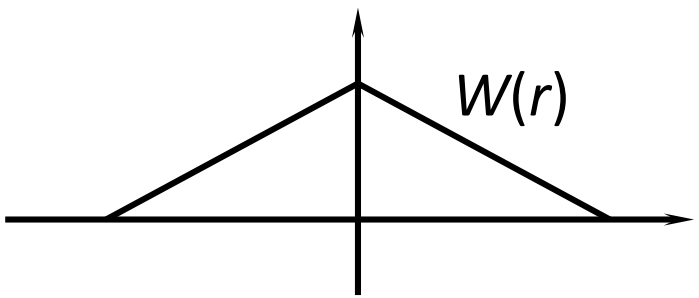


Locality

Additivity

$$\nabla f\big|_a = D\sum_i \frac{f_{ia}}{r_{ai}^{\,2}} r_{ai} \frac{m_i}{\rho_i} W_{ai}$$

$$\Delta f\big|_a = 2D\sum_i \frac{f_{ia}}{r_{ai}^{\,2}} \frac{m_i}{\rho_i} W_{ai}$$

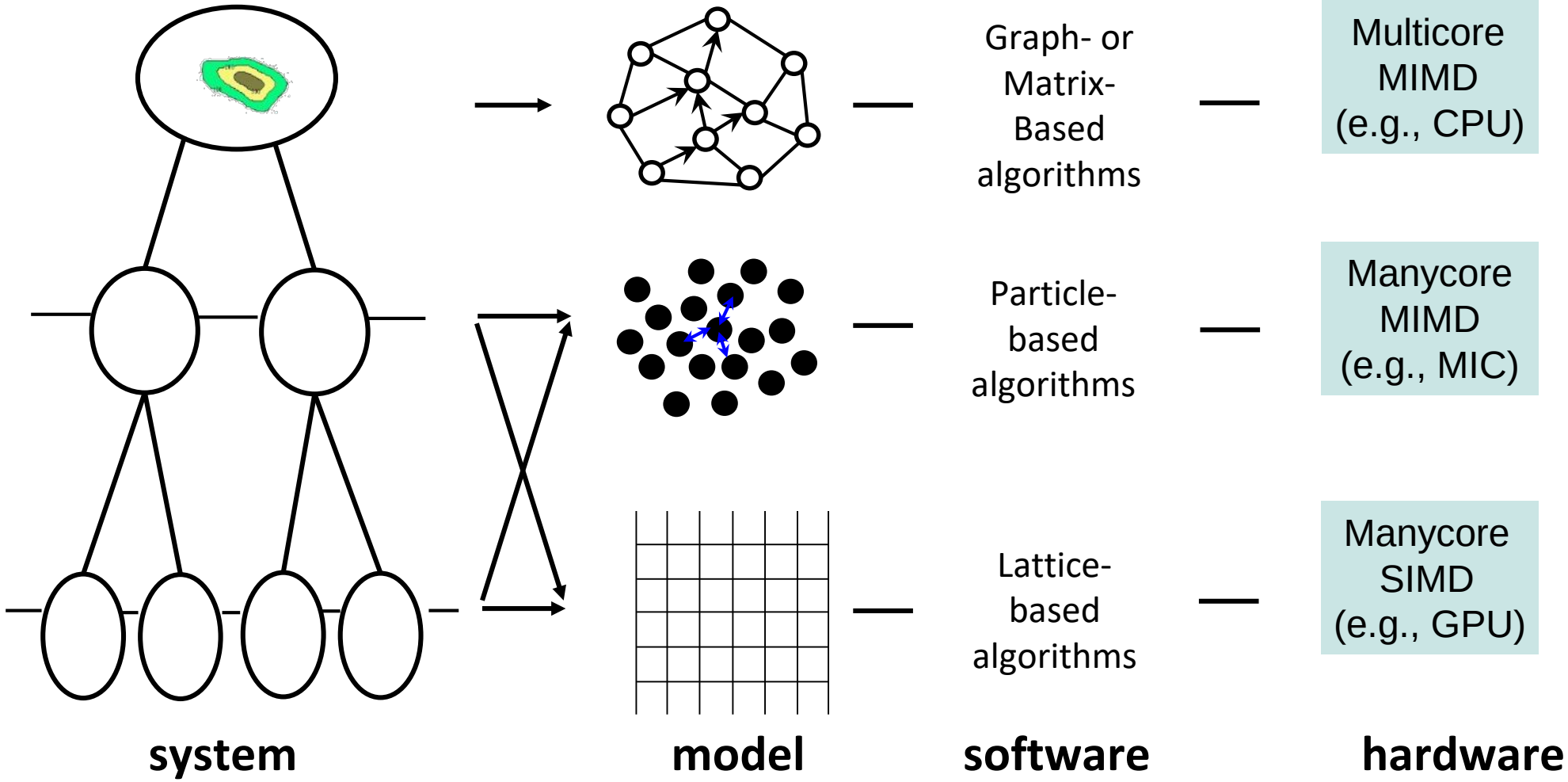


Similarity

MD MC PPM, DPD LBM, …
DEM SPH PIC MaPPM, CG-DEM, …

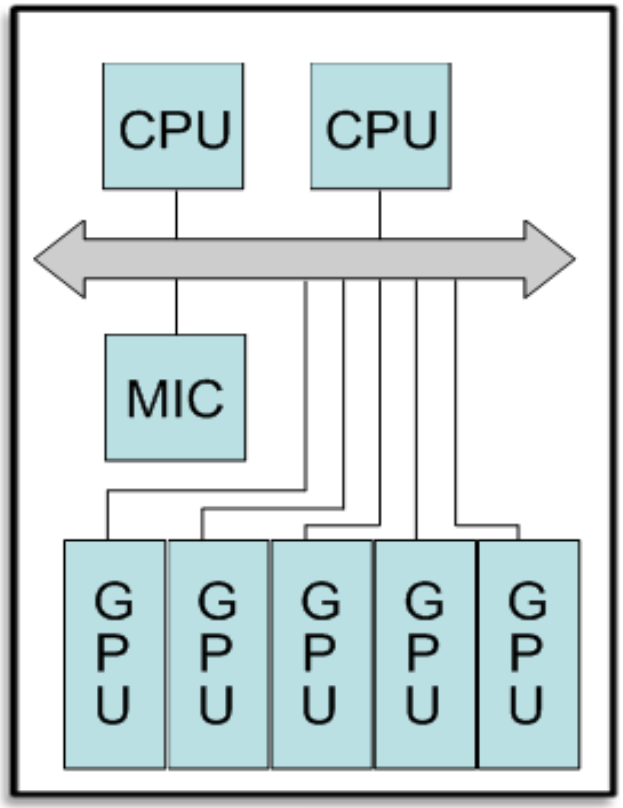
Xu et al. 2015 *Chem. Eng. Sci.* 121:200-216

Software-hardware co-design



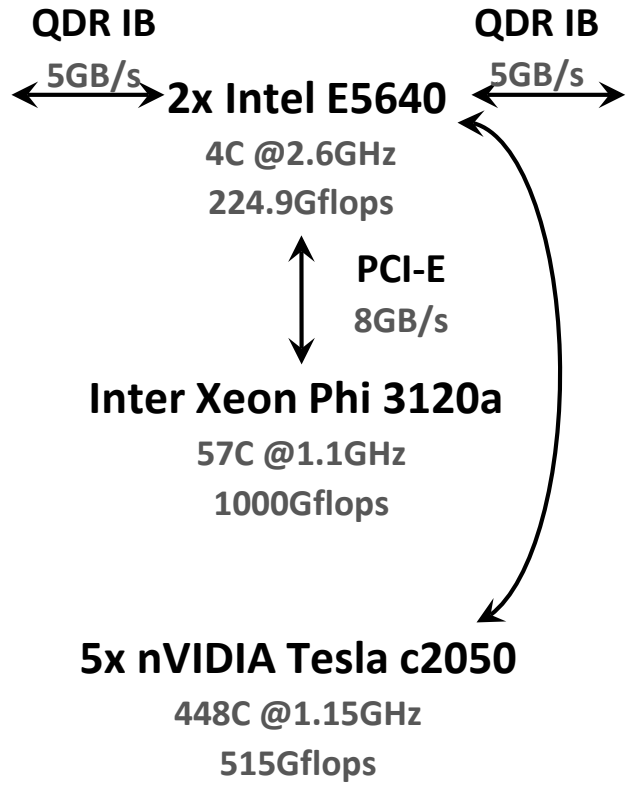
Ge et al. 2015 *Chem. Eng. & Tech.* 38:575-584

Multi-scale node architecture



Architecture

Layout



Configuration

Li et al. 2014 *Particuology* 15:160-169; Ge et al. 2015 *Chem. Eng. & Tech.* 38:575-584

Greenest petaflops supercomputer in 2010

Rpeak SP:	2.26Petaflops ~ $10^{-8.5}$ Mole-flops
Rpeak DP:	1.13Petaflops
Linpack:	496.5Tflops (19th, Top500, 2010)
Mflops/Watt:	963.7 (8th, Green500, 2010)
memory:	17.2TB (RAM), 6.6TB (VRAM)
storage:	76TB (Nastron)+320TB (HP)
network:	Mellanox QDR InfiniBand
occupied area:	150m^2 (with internal cooling)
weight:	12.6T (with internal cooling)
max power:	600kW+200kW (cooling)

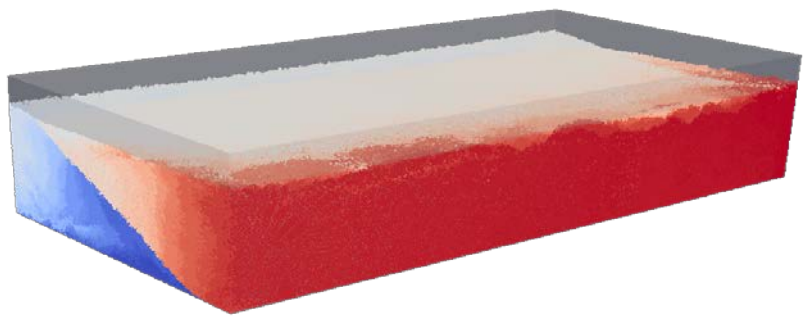
GPU performance in DEM simulation

Configuration

Cases	$N_{particles}$
1	7,220
2	120,159
3	240,318
4	480,636
5	961,274
6	1,922,548
7	3,845,096

Parameters

- State: compact packing (most colliding neighbors)
- Box： 80×40 ×20 m^3
- Radius of particles: 12.5 mm
- Time step: 10^{-4} s
- Grid size: 2 times of diameter of particles
- Neighbor searching cutoff: 2 times of diameter of particles
- Average neighboring particles in neighbor list: ~20



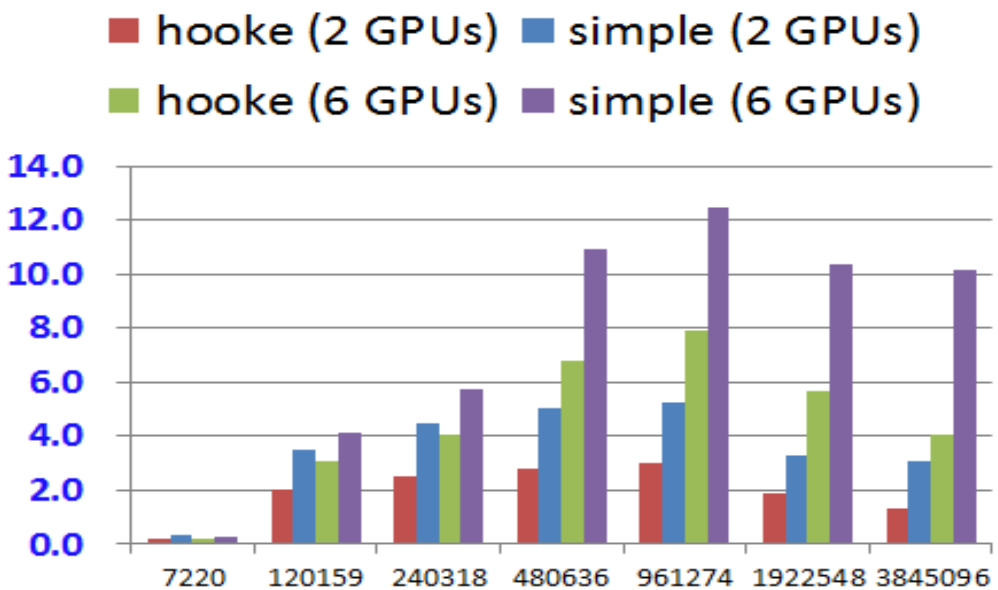
packing state

Xu et al. 2016 *IPE Internal Report*

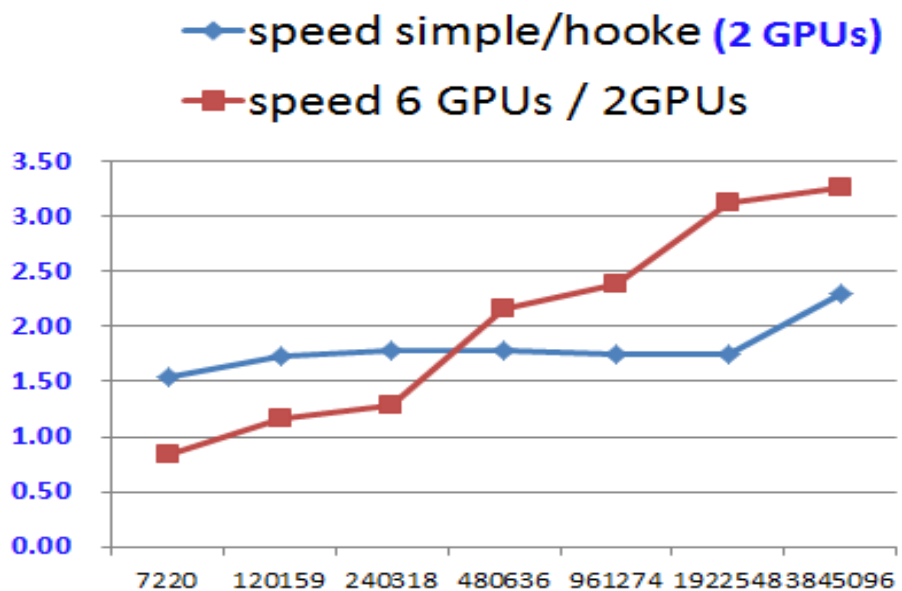
GPU performance in DEM simulation

Speed of different models

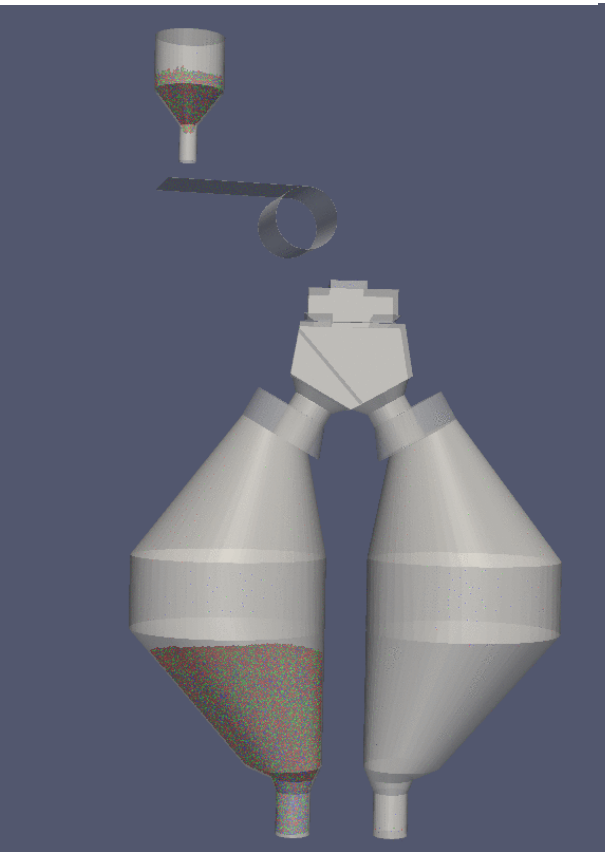
$N_{particle}*N_{step}/time\ (10^8)$



Relative speed

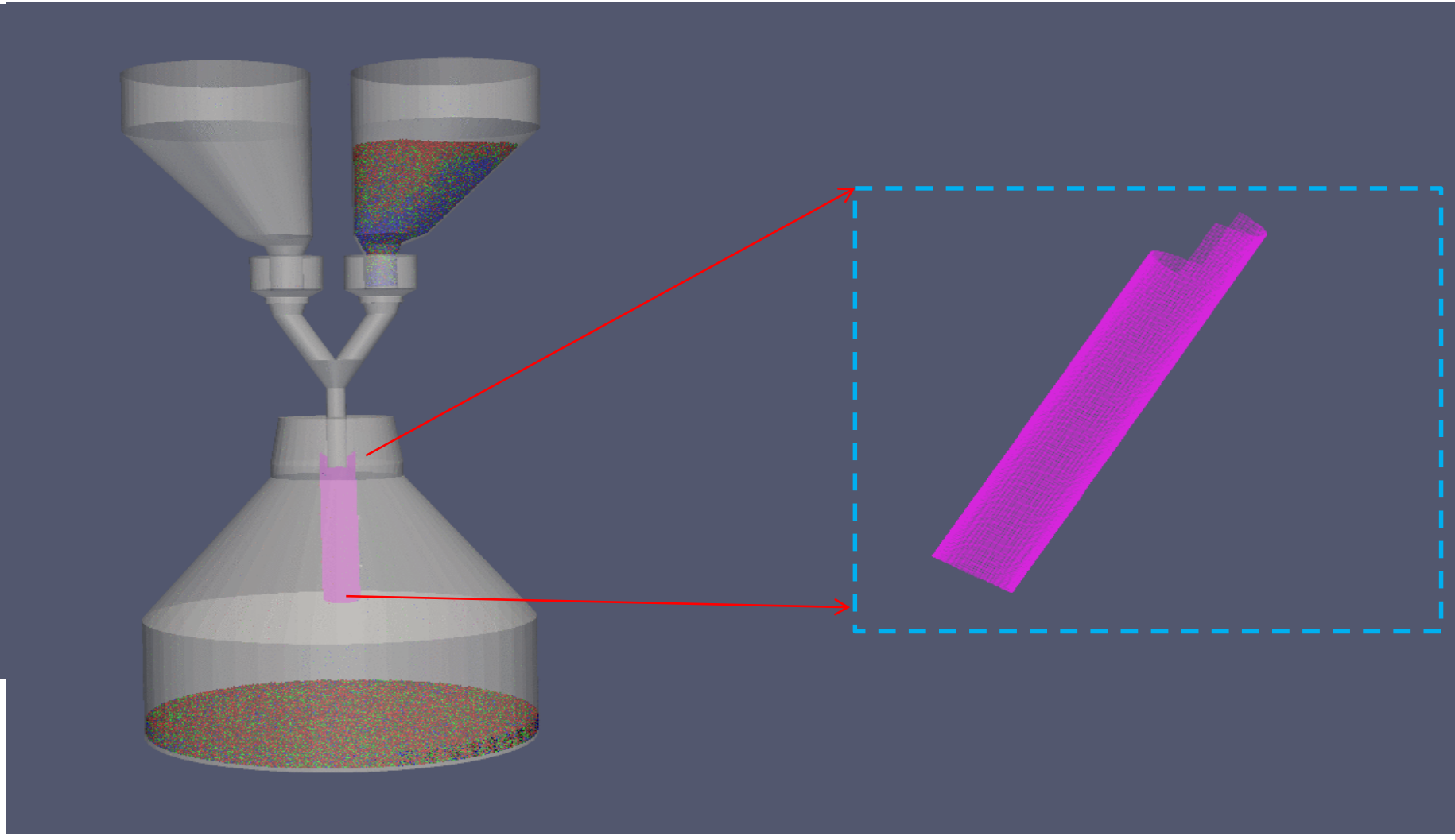


Full scale simulation of a blast furnace



storage

distribution

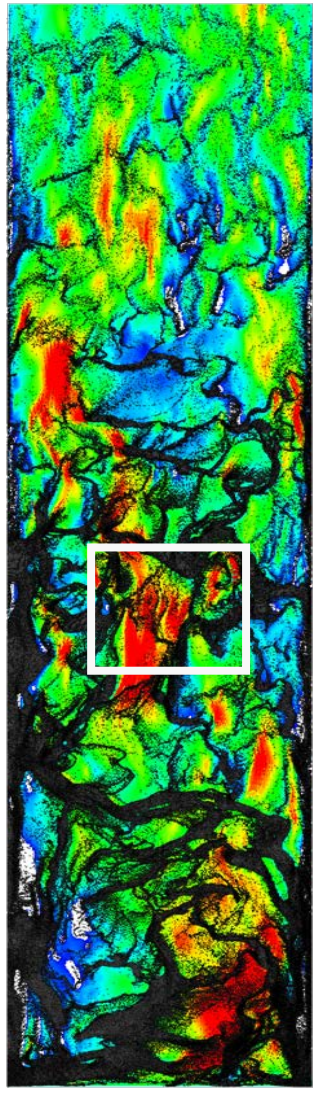


Ren et al. 2015 *Internal Report*

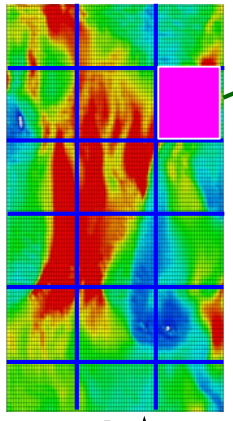
Example I

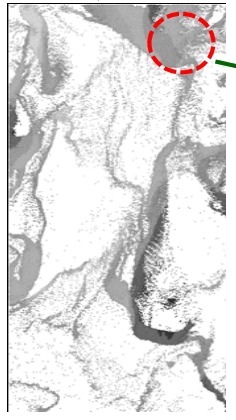
Discrete particle simulation of gas-solid flow

CFD-DEM method



fluid phase





solid phase

Navier-Stokes equation

mass conservation

$$\frac{\partial\left(\varepsilon\rho_{\mathrm{g}}\right)}{\partial \mathrm{t}}+\nabla\cdot\left(\varepsilon\rho_{\mathrm{g}}\mathbf{u}\right)=0$$

momentum conservation

$$\frac{\partial\left(\varepsilon\rho_{\mathrm{g}}\mathbf{u}\right)}{\partial t}+\nabla\cdot\left(\varepsilon\rho_{\mathrm{g}}\mathbf{u}\mathbf{u}\right)=-\varepsilon\nabla p+\nabla\cdot\left(\varepsilon\boldsymbol{\tau}\right)+\varepsilon\rho_{\mathrm{g}}\mathbf{g}+\mathbf{F}_{d}$$

coupling

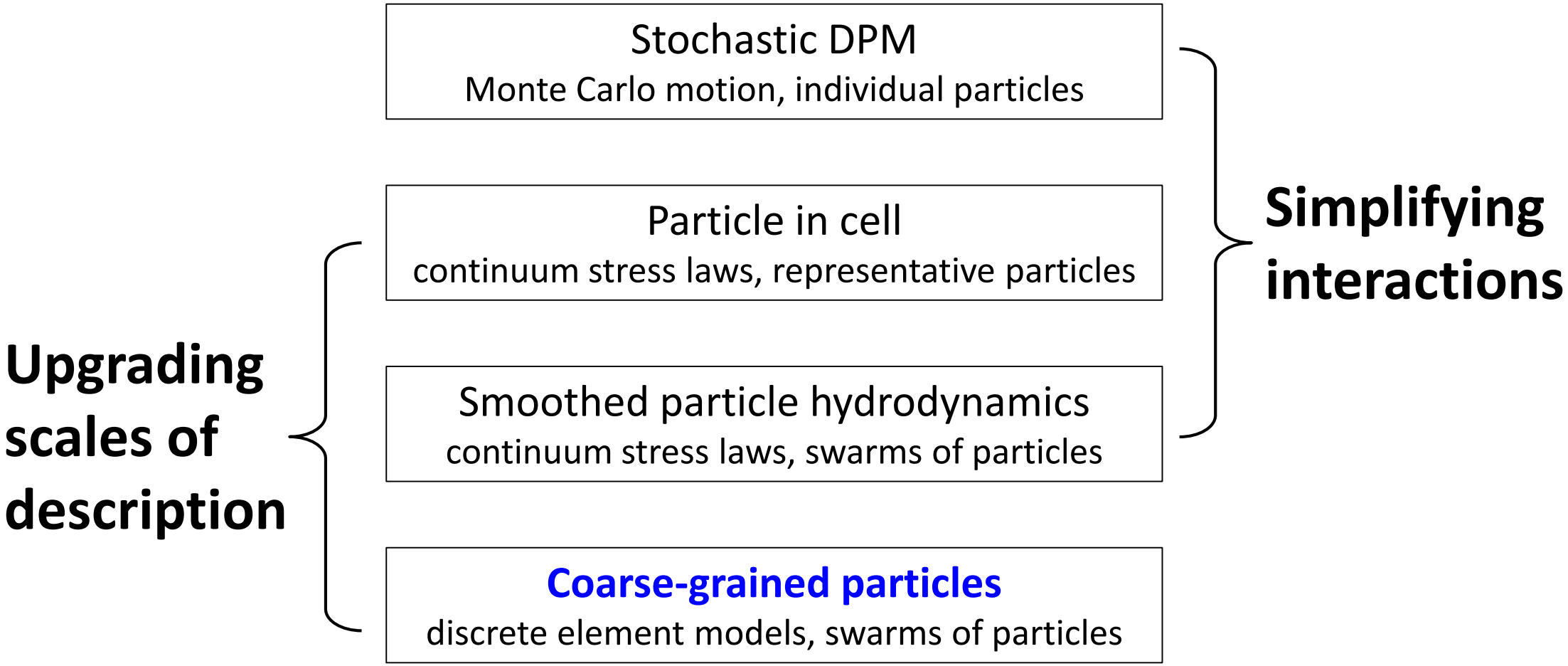
$$\mathbf{F}_{d}=-\frac{1}{V_{\mathrm{cell}}}\sum_{i\in\mathrm{cell}}\mathbf{f}_{i}^{d}$$

discrete element method

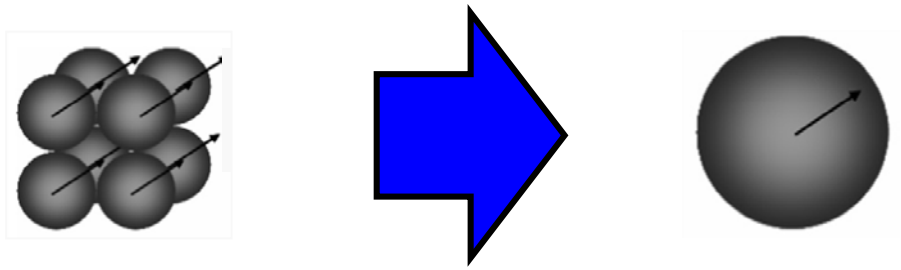
$$m_i\frac{d\mathbf{v}_i}{dt}=\sum_j\mathbf{f}_{ij}^{c}+\mathbf{f}_i^{d}+m_i\mathbf{g}$$

$$I_i\frac{d\boldsymbol{\omega}_i}{dt}=\sum_j\mathbf{T}_{ij}$$

More efficient discrete methods



Development of coarse-grained models



The k^3 real particles are represented by k coarse-grained particles and

$$d_c = k^3 d_0$$

* The modification of micro-dynamics on particles (Similar particles assembly, **SPA**)

$$m_c \frac{d\boldsymbol{v}_{p,c}}{dt} = \boldsymbol{F}_{d,c} - V_c \nabla P + \sum \boldsymbol{F}_c + \boldsymbol{G}_c$$
$$= k^3 (\boldsymbol{F}_{d,0} - V_0 \nabla P + \sum \boldsymbol{F}_{c,0} + \boldsymbol{G}_0)$$

** In addition, the coefficient of restitution is modified as (**MSPA**):

$$\frac{\ln e_c}{\ln e_0} = \sqrt{k^3}$$

* Sakai et al. 2010, Int J Numer Meth Fl. 64:1319-1335

** Benyahia et al. 2010, Ind Eng Chem Res. 49:10588-10605

Development of coarse-grained models

Modification of fluid properties for constant *Re* and *Ar* (Principle of similarity model, **PSM**)

$$\frac{\mu_{g,c}}{\mu_{g,0}} = k^2 \qquad \frac{\rho_{g,c}}{\rho_{g,0}} = k$$

$$\boldsymbol{G_c} = \rho_{p,c}\frac{1}{6}\pi d_c^3\mathbf{g} = k^3\rho_{p,0}\frac{1}{6}\pi d_0^3\mathbf{g} = k^3\boldsymbol{G_0}$$

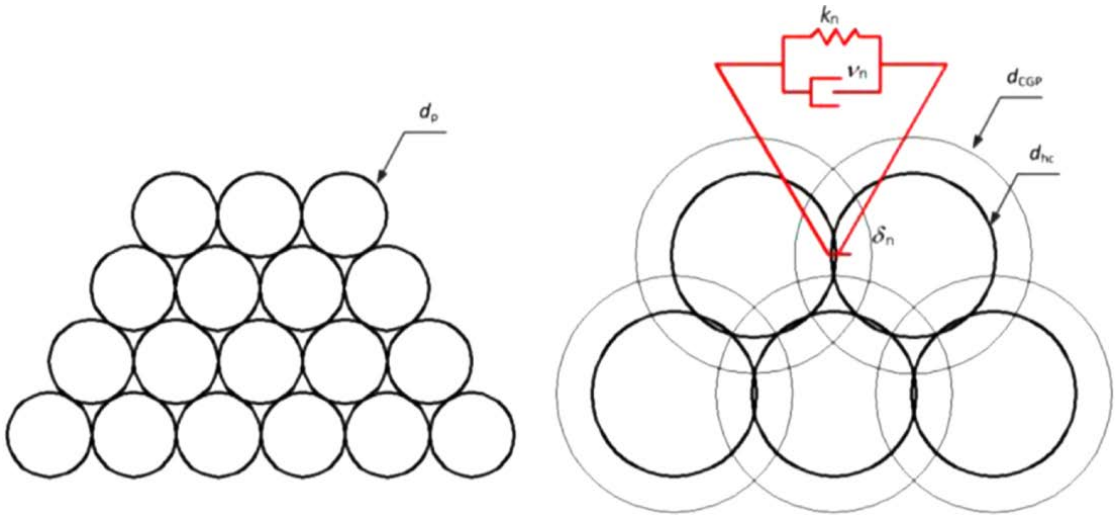
$$\mathbf{F_{g,c}} = \left(\frac{\beta_c}{1-\varepsilon_c}(\boldsymbol{u_{g,c}} - \boldsymbol{v_{p,c}}) - \nabla \mathrm{P}\right)V_c = \left(\frac{\beta_0}{1-\varepsilon_0}(\boldsymbol{u_{g,0}} - \boldsymbol{v_{p,0}}) - \nabla \mathrm{P}\right)k^3V_0 = \mathrm{k}^3\mathbf{F_{g,0}}$$

$$\mathrm{Umf_c} = \frac{\mu_{g,c}}{\rho_{g,c}d_c}f(\mathrm{Ar}) = \frac{k^2\mu_{g,0}}{k^2\rho_{g,0}d_0}f(\mathrm{Ar}) = \mathrm{Umf_0}$$

No change to the particle-particle interactions

*Liu et al. 2013, 14th International Conference on Fluidization .

Coarse-graining with statistical equivalence



$k^3(1-\varepsilon_{CGP})$ real particles are lumped into k coarse-grained particles with

$$d_c = k^3 d_0$$

$$\boldsymbol{G_c} = k^3(1-\varepsilon_{CGP})\boldsymbol{G_0}$$

$$d_{hc} = d_c(1-\varepsilon_{CGP})^{1/3}$$

$$\boldsymbol{F_{gra,c}} = -\left(\sum_{i=1}^{N_{n,CGP}} \frac{1}{6}\pi d_c^3\right)\nabla P = -(1-\varepsilon_{CGP})k^3\frac{\pi}{6}d_0^3\nabla P$$

$$e_c = \sqrt{1+k(e_0^2-1)(1-\varepsilon_{CGP})^{1/3}}$$

$$\boldsymbol{F_{d,c}} = \frac{\beta_{EMMS}}{1-\varepsilon_{CGP}}(\boldsymbol{u_g}-\boldsymbol{v_{CGP}})V_{CGP}$$

Lu et al. 2014 *Chem. Eng. Sci.* 120:67-87

Derivation of the coefficient of restitution

Kinetic energy loss:

$$\Delta E = \frac{1}{4} m(e^2 - 1)(\mathbf{k} \cdot \mathbf{v}_{\mathrm{r}})^2$$

Collision frequency:

$$f_{\mathrm{c}} = 4n^2 d^2 \sqrt{\pi \Theta} g_0(\varepsilon_{\mathrm{g}})$$

Original system:

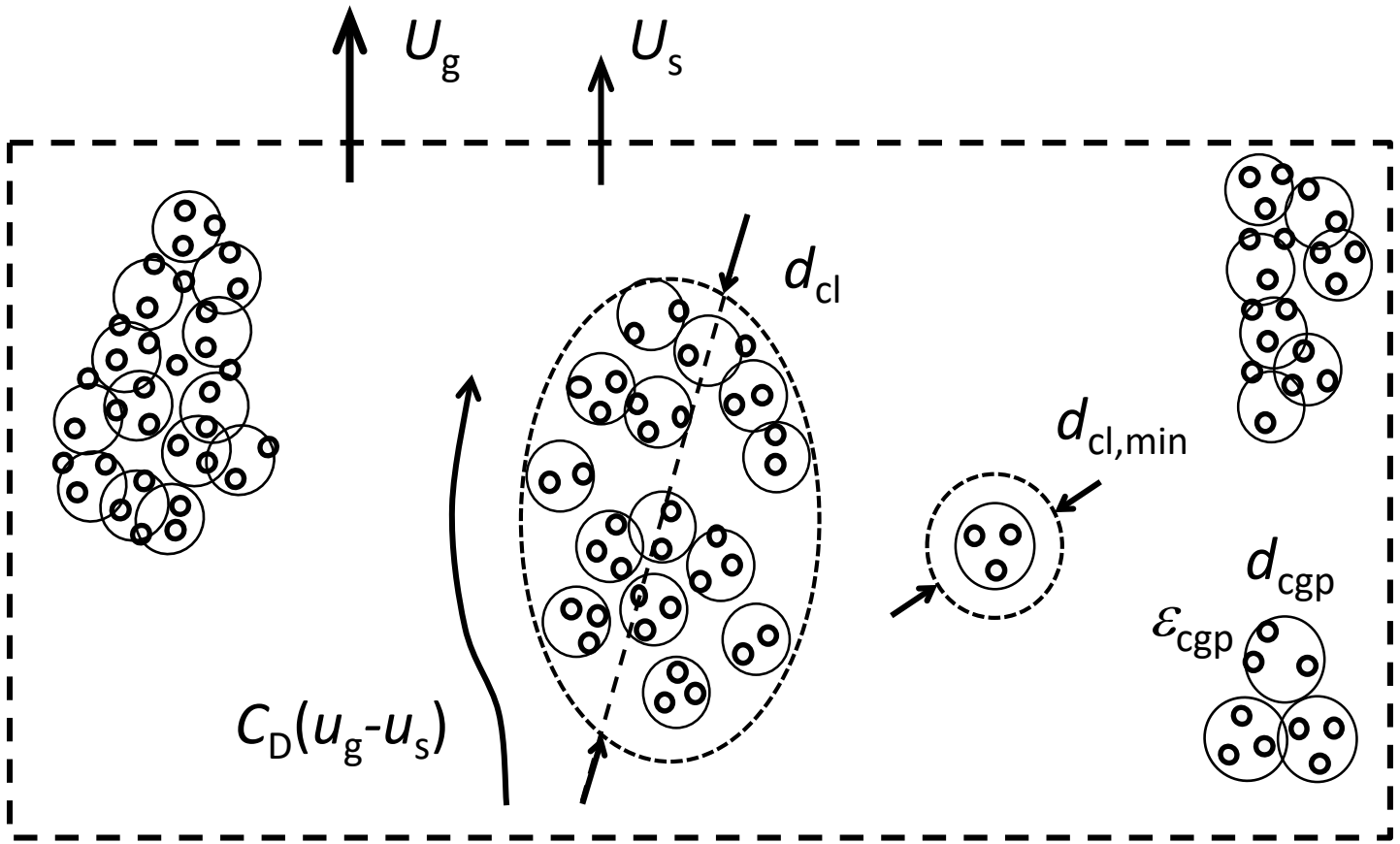
$$\Delta E_{\mathrm{s,p}} = \Delta E \cdot f_{\mathrm{c}} \cdot V_{\mathrm{sys}} = m_{\mathrm{p}} N_{\mathrm{p}}^2 d_{\mathrm{p}}^2 (e_{\mathrm{p}}^2 - 1) \overline{\left| \mathbf{k} \cdot \mathbf{v}_{\mathrm{r,p}} \right|^2} \sqrt{\pi \Theta}_{\mathrm{p}} g_0(\varepsilon_{\mathrm{g}})$$

Coarse-grained system:

$$\Delta E_{\mathrm{s,CGP}} = m_{\mathrm{CGP}} N_{\mathrm{CGP}}^2 d_{\mathrm{hc}}^2 (e_{\mathrm{CGP}}^2 - 1) \overline{\left| \mathbf{k} \cdot \mathbf{v}_{\mathrm{r,CGP}} \right|^2} \sqrt{\pi \Theta_{\mathrm{CGP}}} g_0(\varepsilon_{\mathrm{g}})$$

$$e_{\mathrm{CGP}} = \sqrt{1 + (e_{\mathrm{p}}^2 - 1) k (1 - \varepsilon_{\mathrm{CGP}})^{1/3}}$$

Critical parameters from EMMS



Structure:

$d_{cl,min} > d_{cgp}$

↑

EMMS

↓

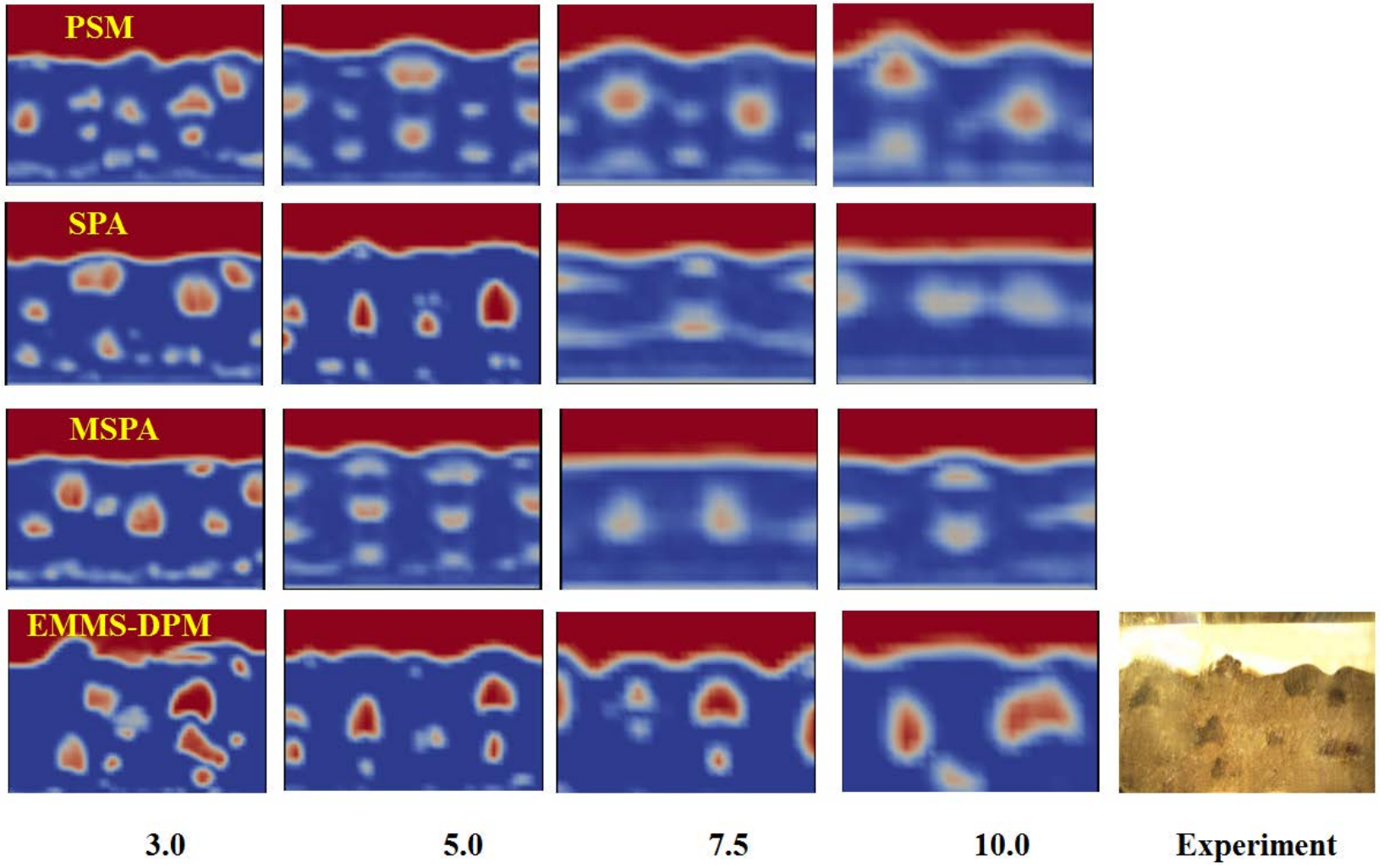
$\varepsilon_{cl,max} > \varepsilon_{cgp}$

Drag:

$C_{D,cgp}=C_{D,EMMS}$

Lu et al. 2014 *Chem. Eng. Sci.* 120:67-87

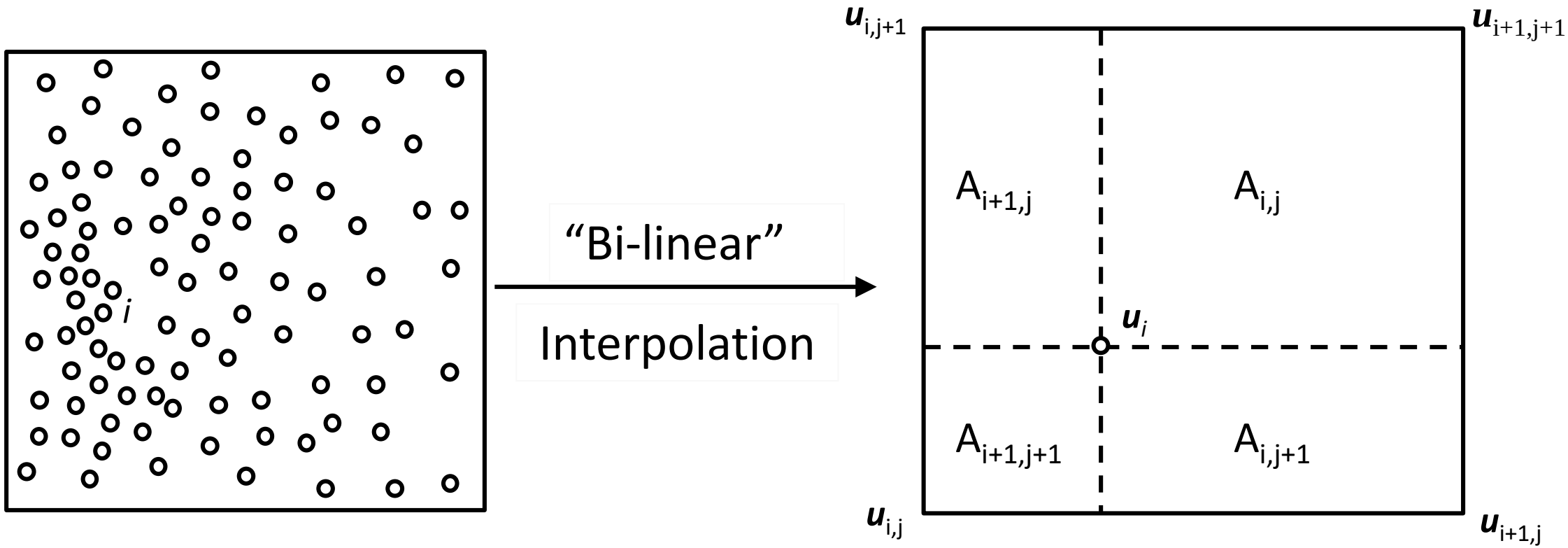
Simulation of a bubbling fluidized bed



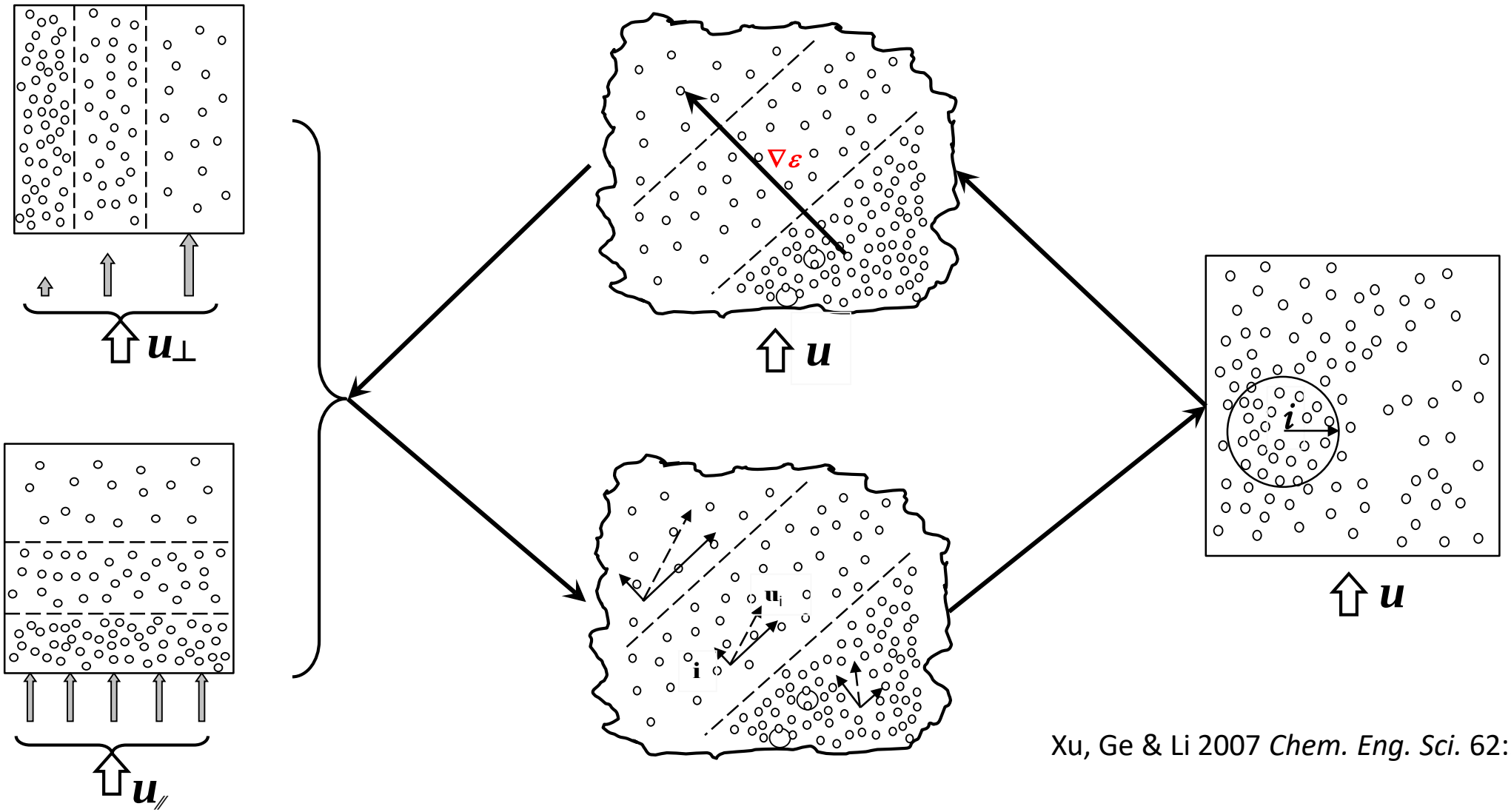
Zhang et al. 2017. Submitted to *Powder Tech.*

Flow distribution

Traditional approach ignores meso-scale structure

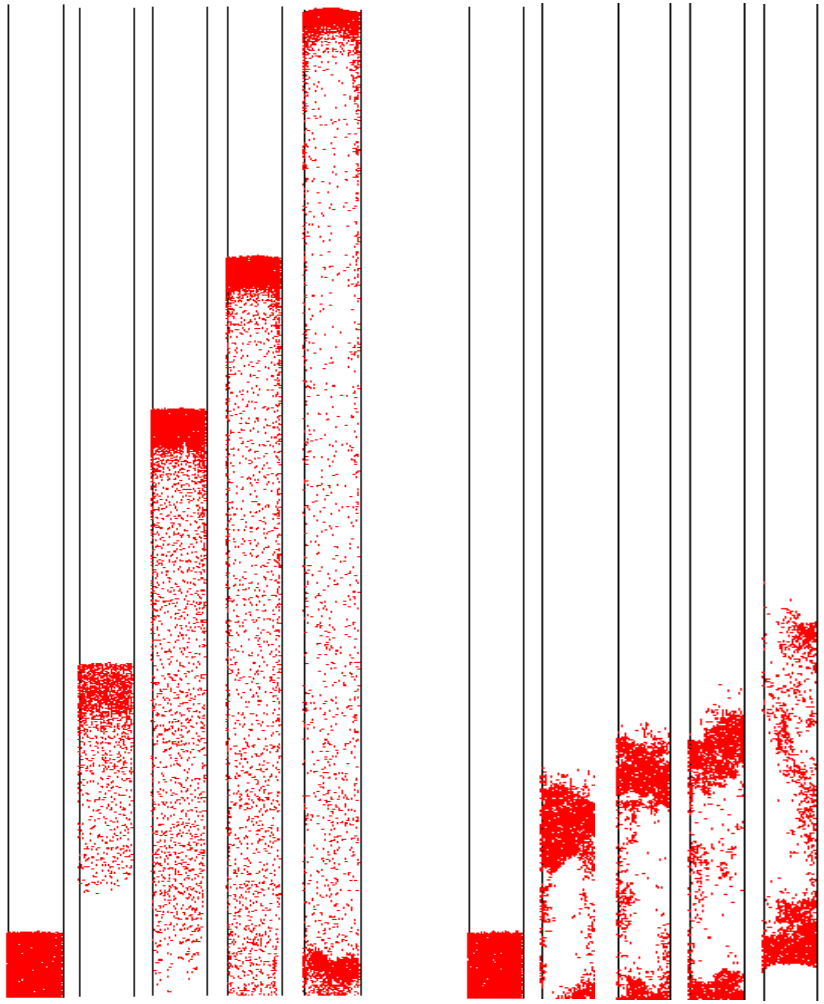


Structure-based flow distribution

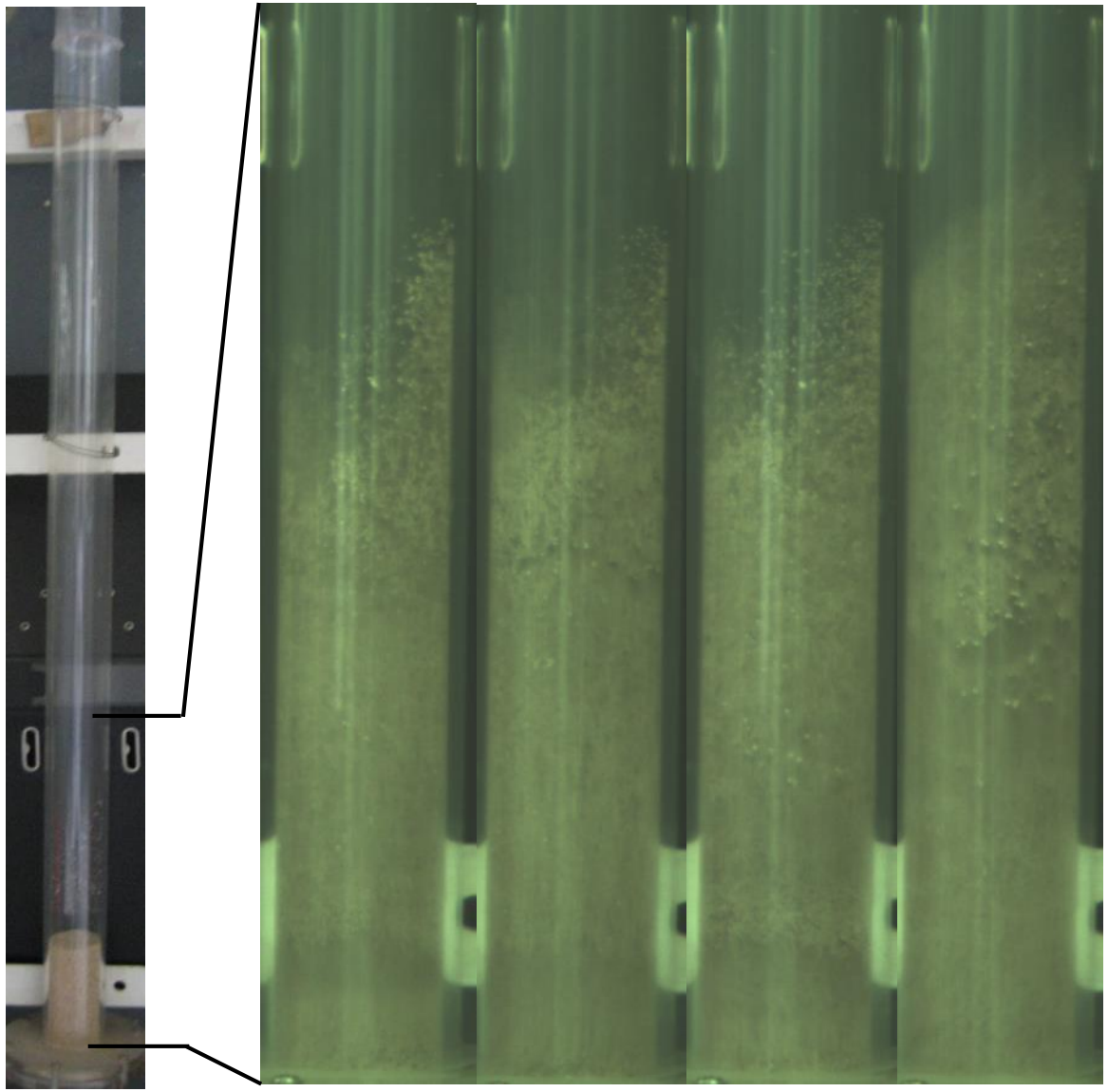


Xu, Ge & Li 2007 *Chem. Eng. Sci.* 62:2302

Slugging: simulation vs experiment

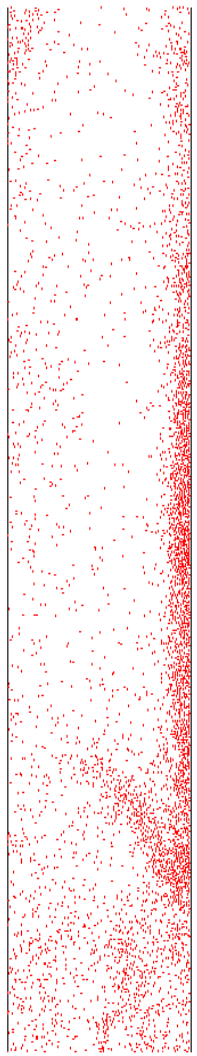


DPM only DPM+EMMS

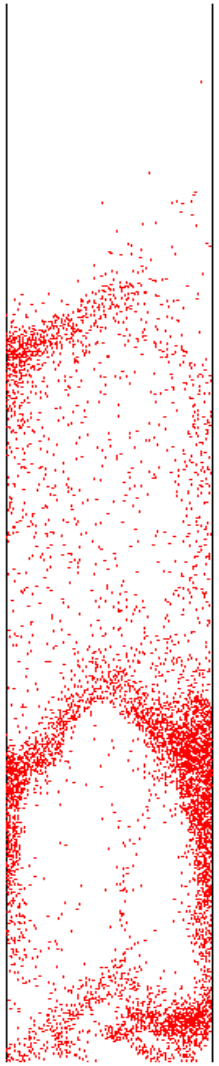


Xu, Ge & Li 2007 *Chem. Eng. Sci.* 62:2302

Simulation of lab-scale CFB riser



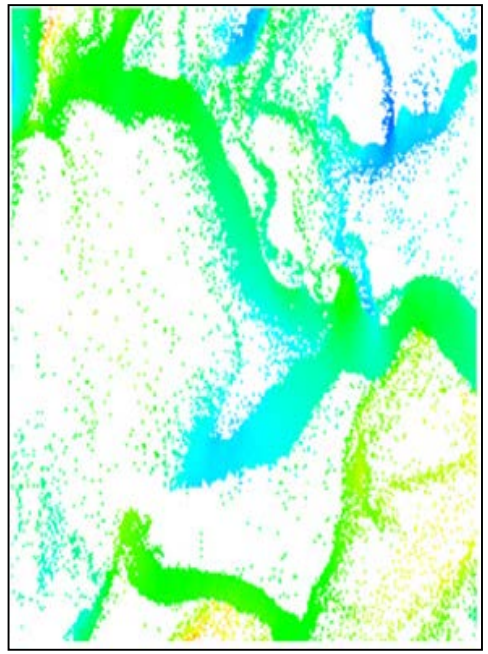
DPM



DPM+EMMS

Experiment:
Chem. Eng. Sci. 49:2413, 1994

Simulation:
Xu et al. 2012 *Chem. Eng. J.* 207:746–757

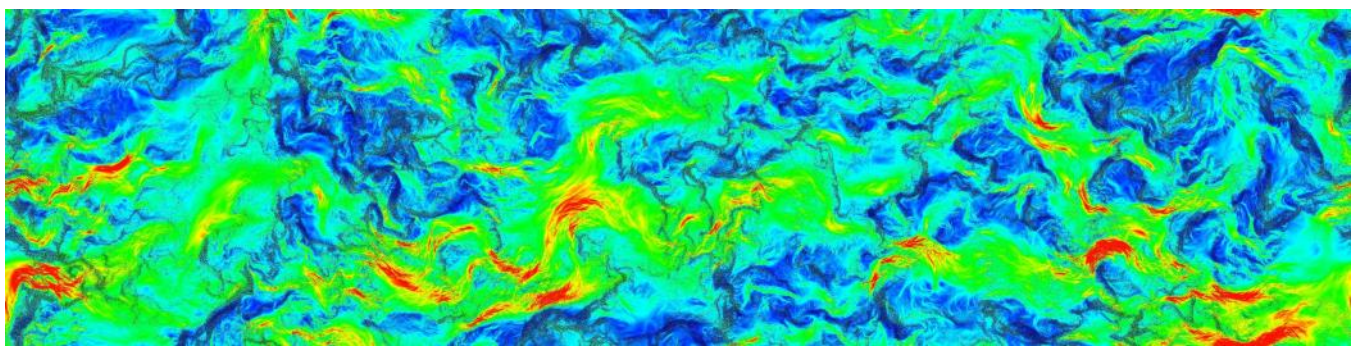


Up to 10 million particles
100mm ID x 6m in 2D, 20x(CPU+GPU)
Speed at ~0.2s per day using ~0.5μs time step

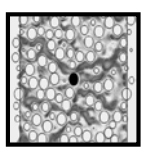
Scale-independent clustering from DNS

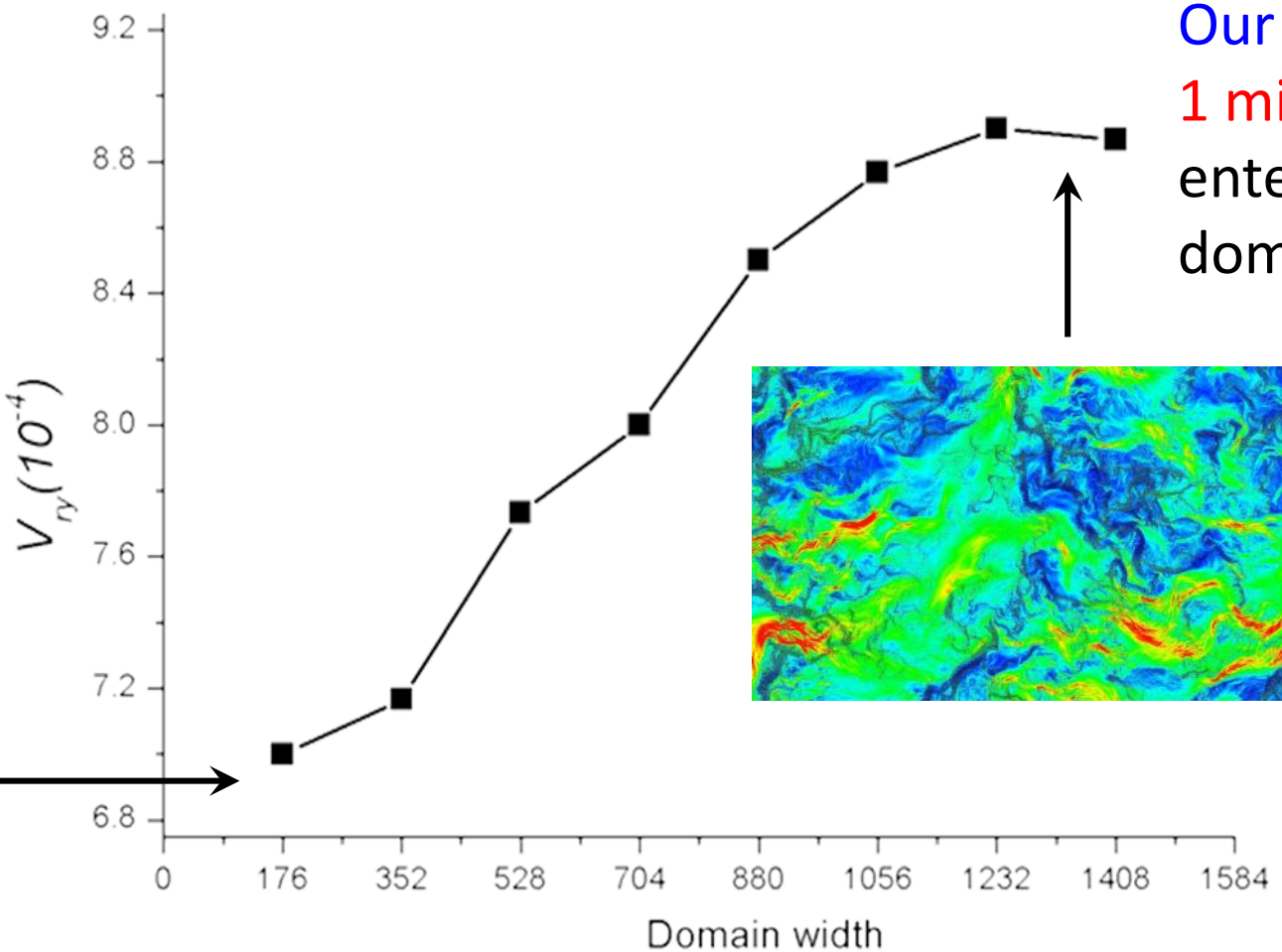
Our results:

1 million particles, 1 billion lattices entering the scale-independent domain for the first time.



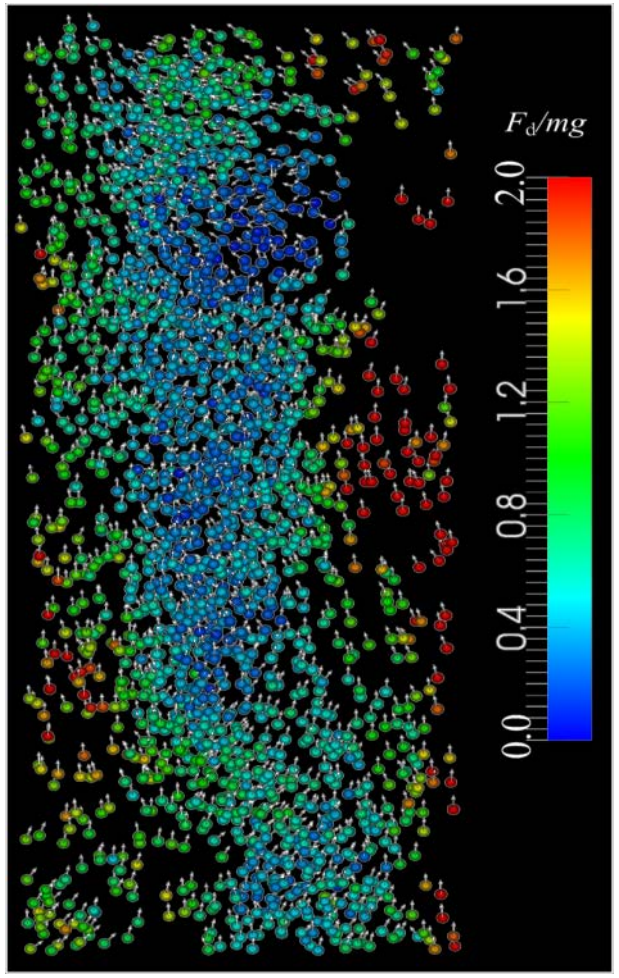
Previous results: ~100 particles





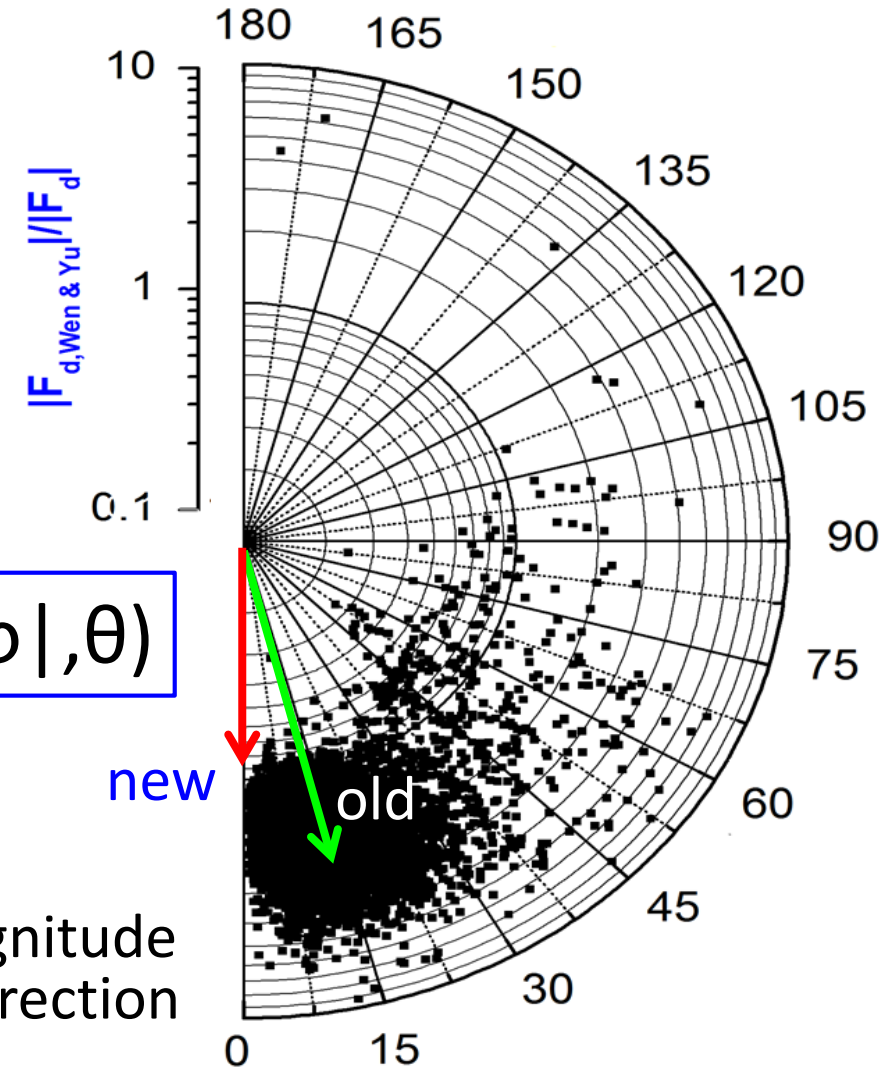
Ge et al. 2011 *Chem. Eng. Sci.* 66:4426-58; Xiong et al. 2012 *Chem. Eng. Sci.* 71:422-430

Drag characteristics revealed by DNS



Spatial distribution

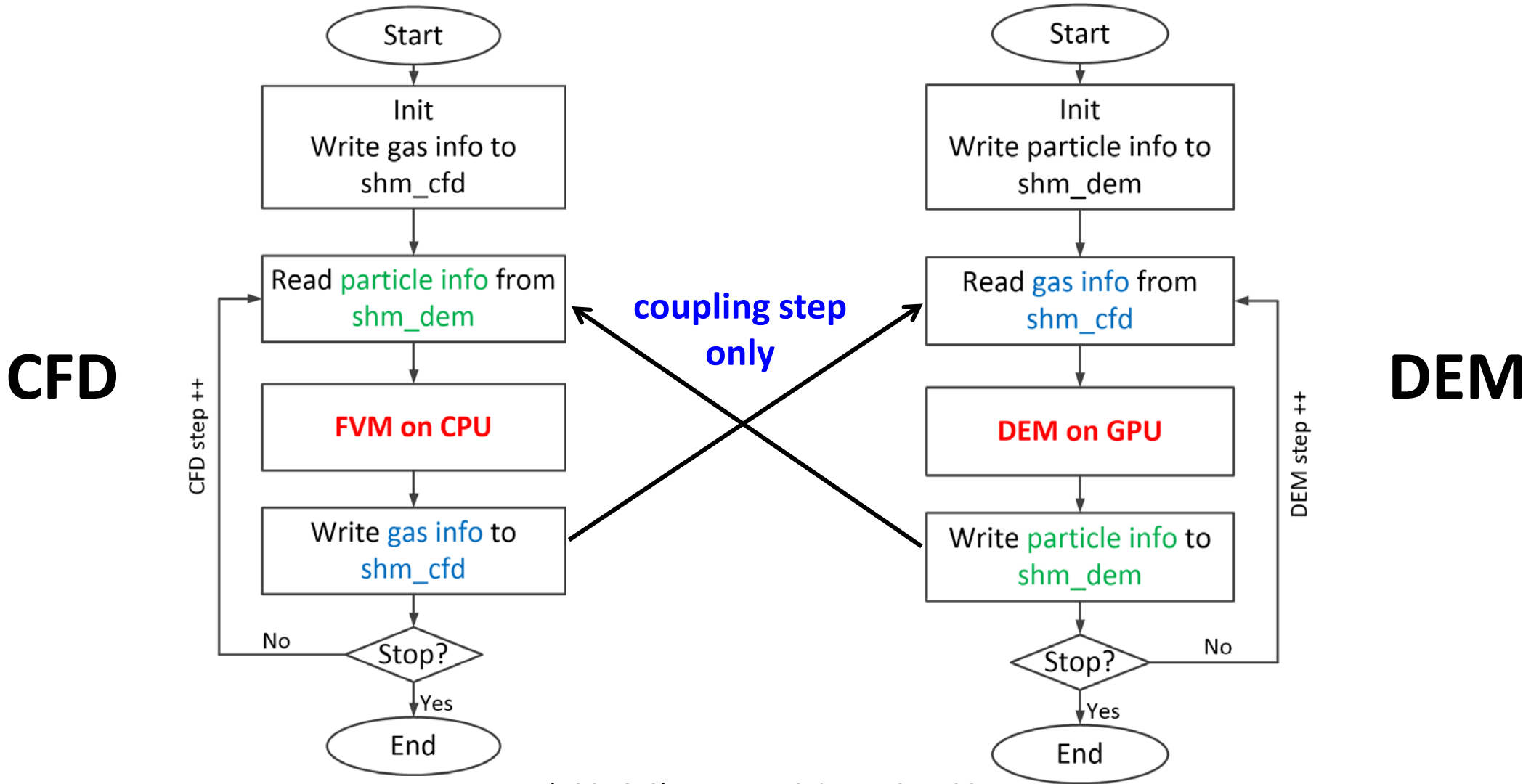
$$F(Re_p, \varphi, |\nabla\varphi|, \theta)$$



Magnitude & direction

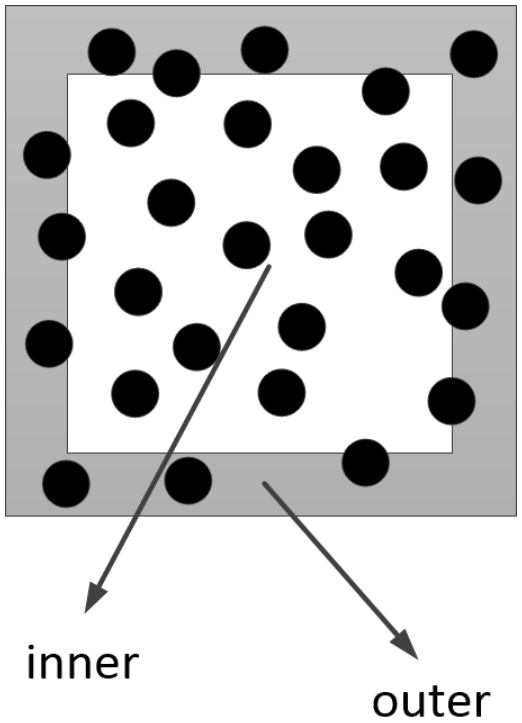
Zhou et al. 2014 *Chem. Eng. Sci.* 116:9-22

Flowchart for CFD-DEM coupling

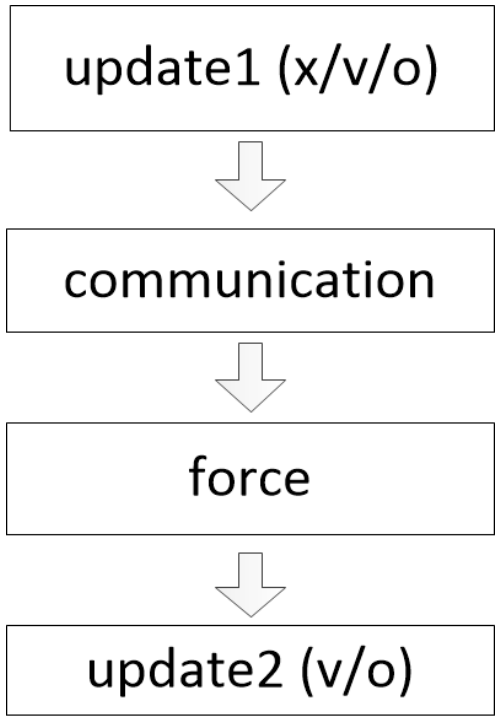


Lu et al. 2016 *Chem. Eng. Sci.* 155:314-337

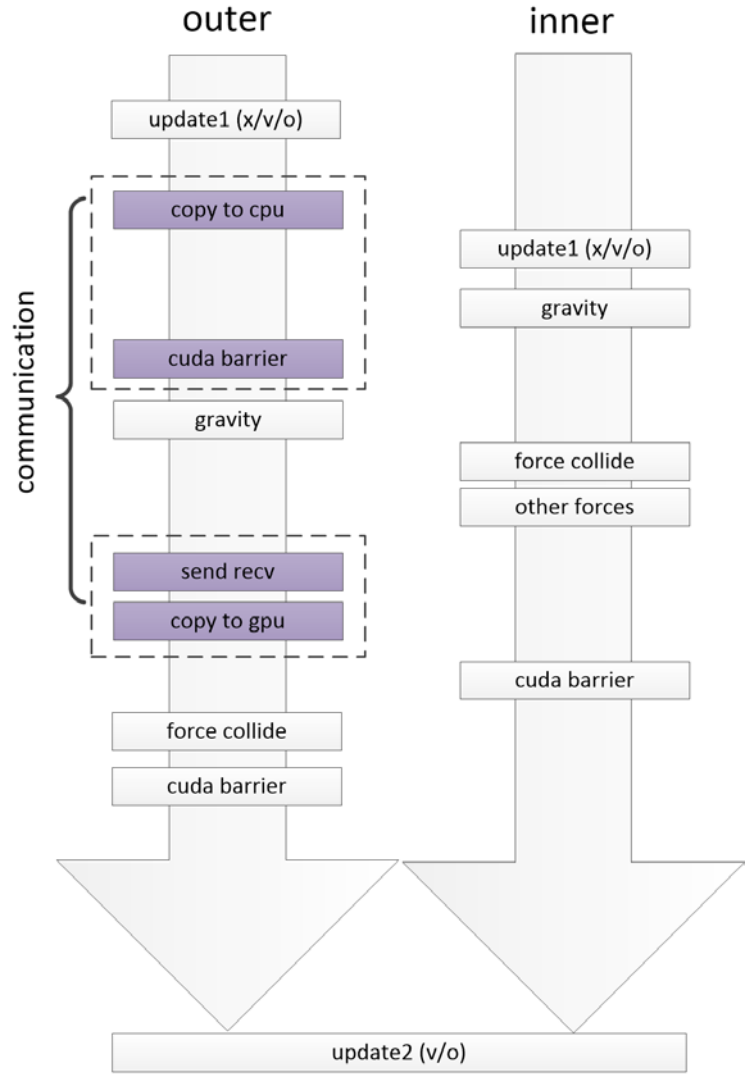
Overlapping of computing & communication



particle order & storage

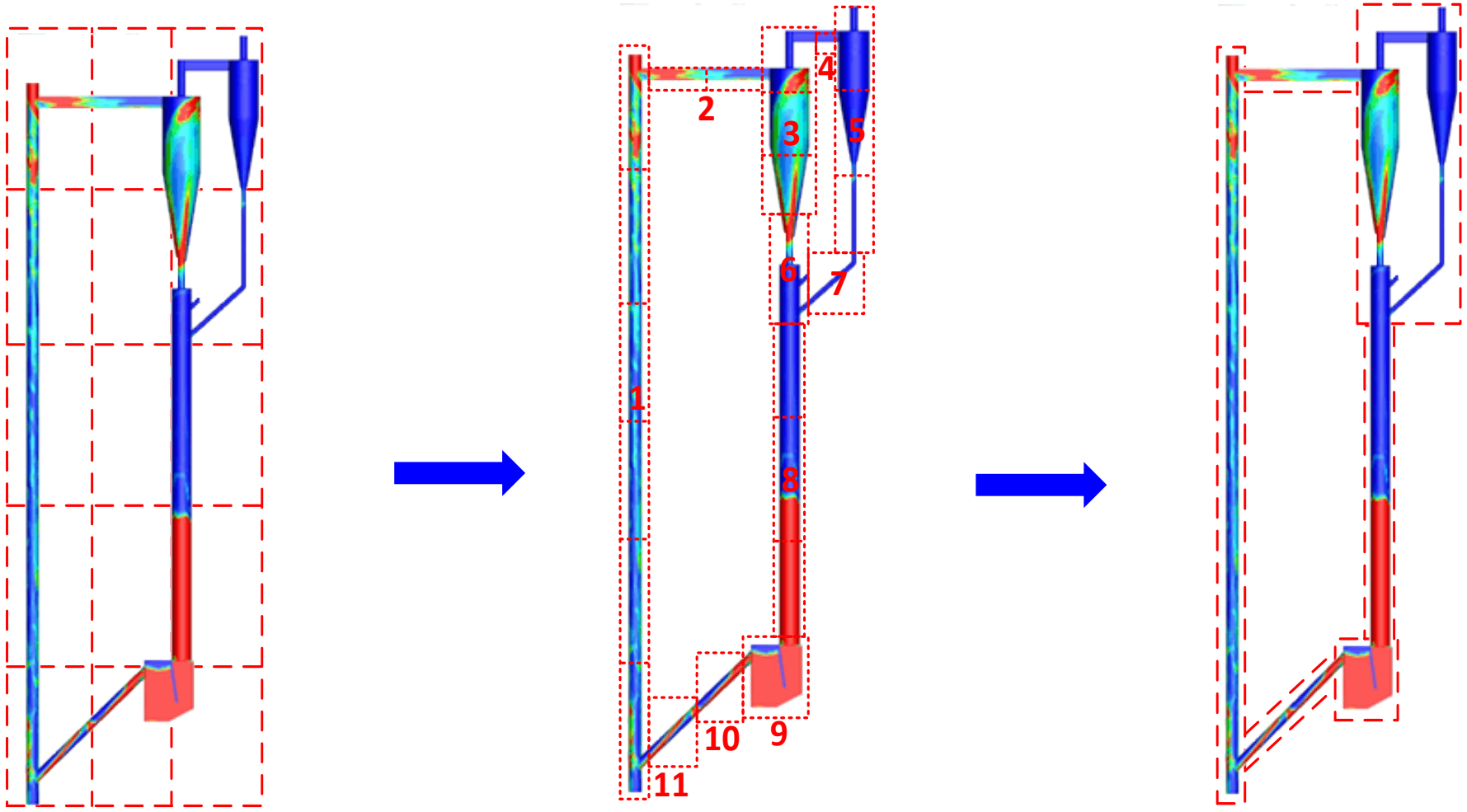


main tasks



Lu et al. 2016 *Chem. Eng. Sci.* 155:314-337;
Xu et al. 2016 Huagong Xuebao 67:14-16 (In Chinese)

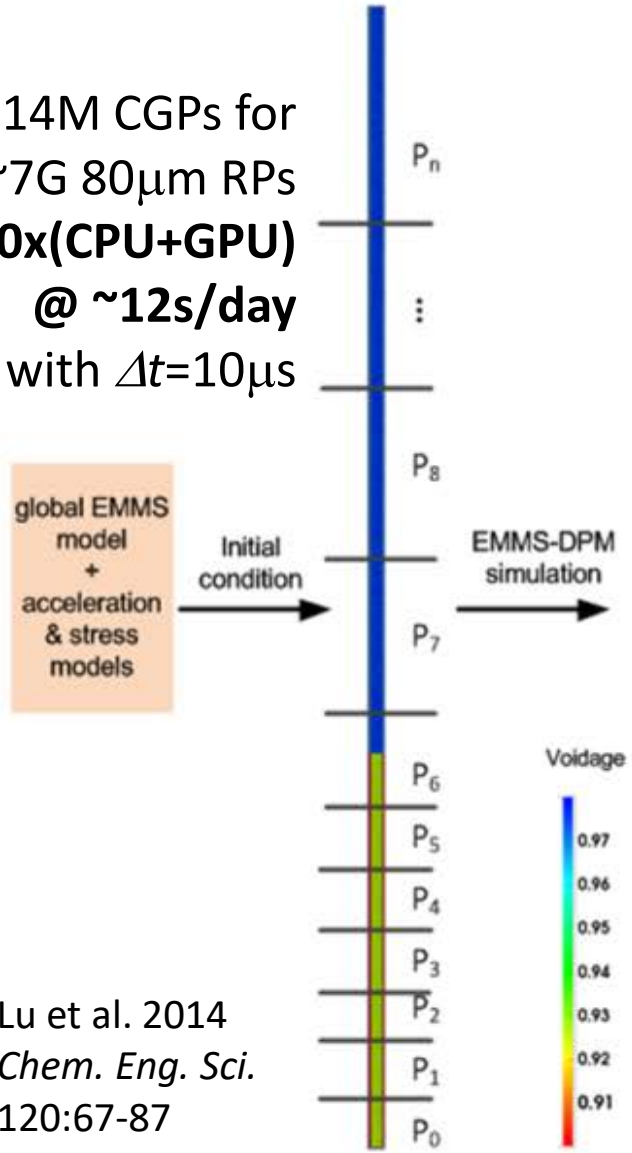
Irregular space decomposition

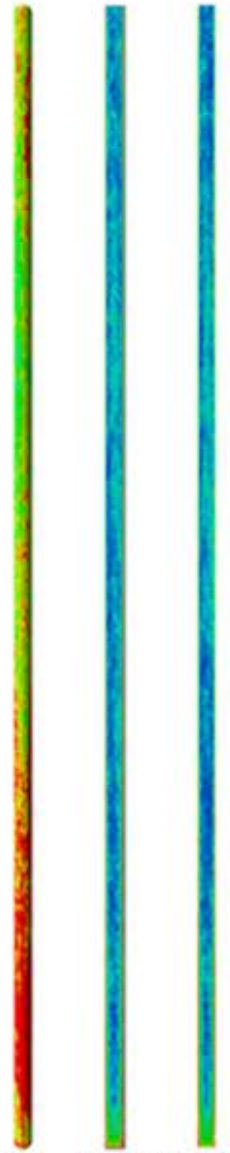


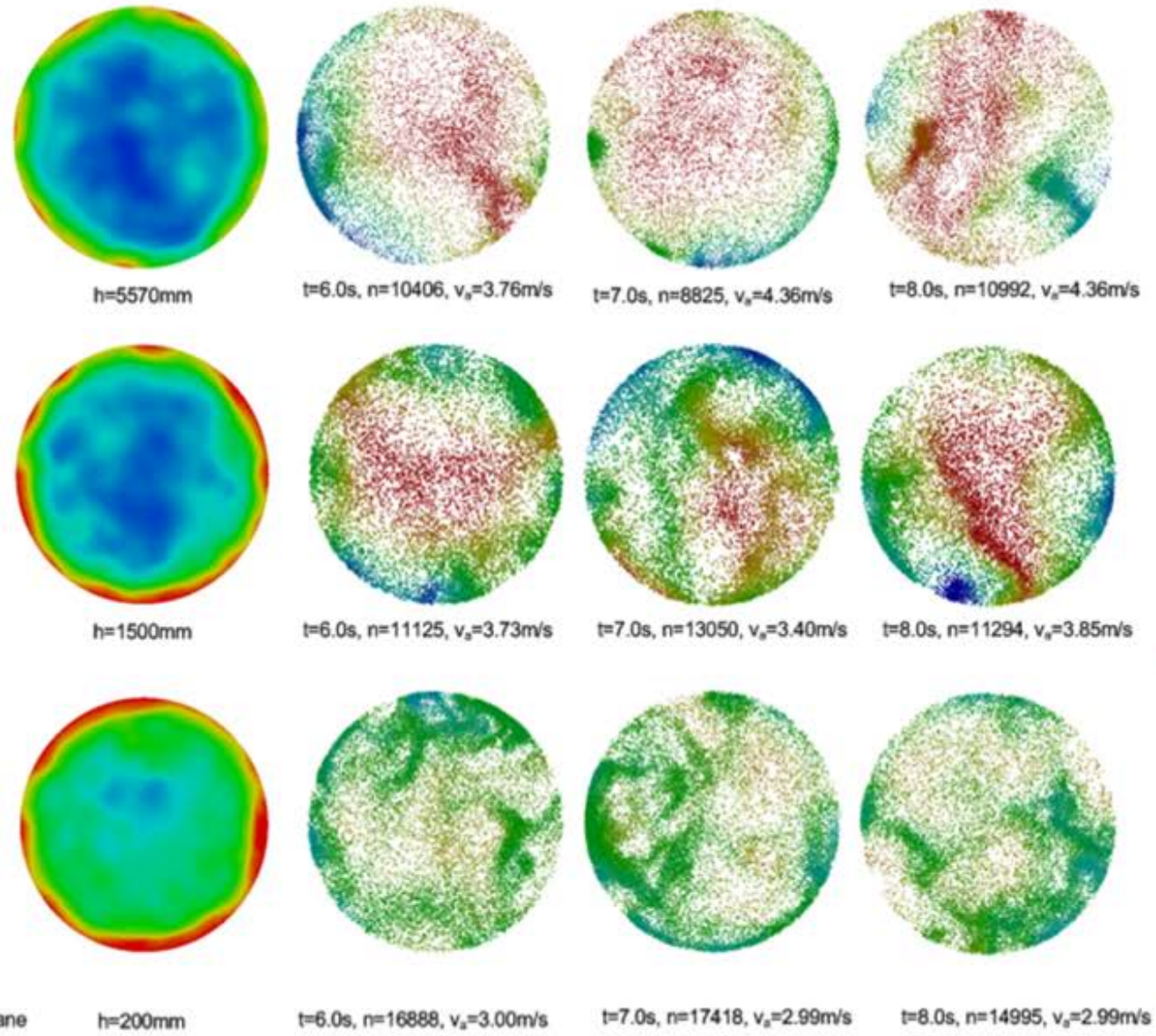
Xu et al. 2016 Huagong Xuebao 67:14-16 (In Chinese); Xu et al. 2017 *IPE Internal Report*

3D simulation of a lab-scale riser in DPM

14M CGPs for
~7G 80μm RPs
120x(CPU+GPU)
@ ~12s/day
with Δt=10μs





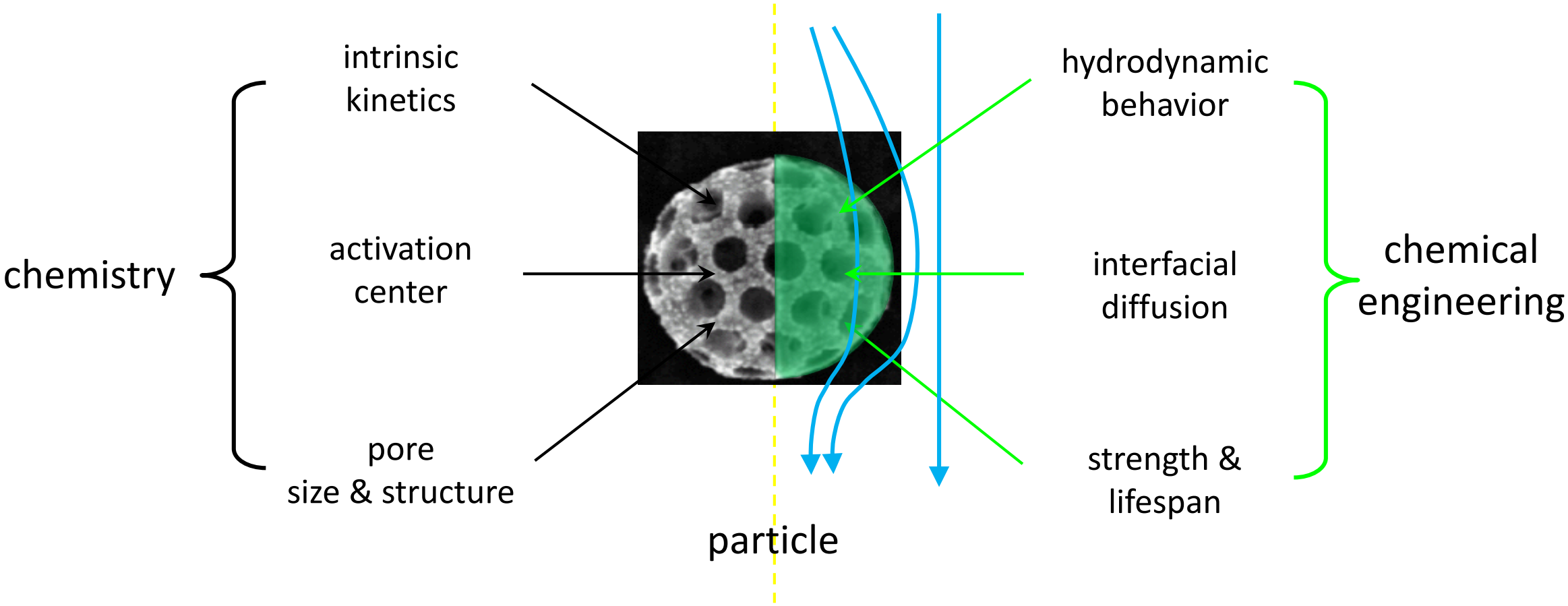


Lu et al. 2014
Chem. Eng. Sci.
120:67-87

Example II

Hard sphere/Pseudo Particle Modeling of high *Kn* flows

Interface of chemistry & chem. eng.



coupled models, concurrent computing

Challenges at the “interface”

- Lack of scale separation
- Strong scale dependence of properties
- Strong non-linear effect (e.g., non-Newtonian, slip…)
- Strong non-equilibrium effect (e.g., anisotropic)

Continuum methods are invalid →

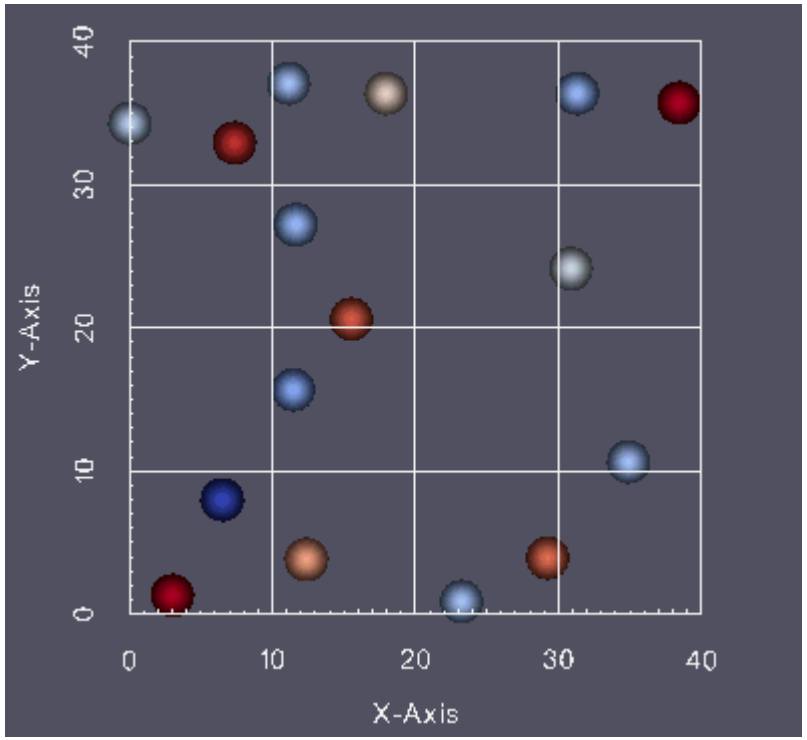
Discrete methods are expensive →

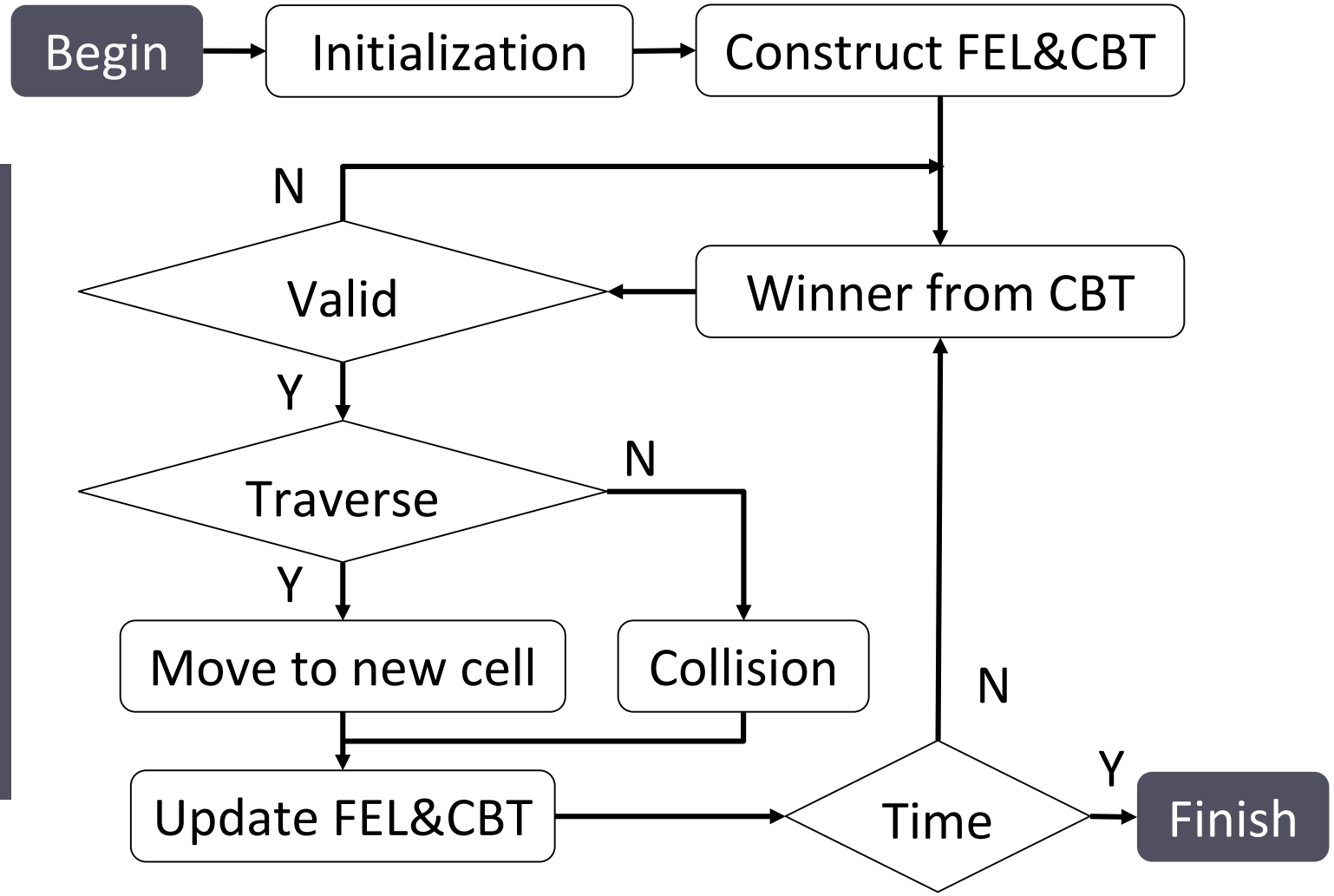
Efficient algorithms & supercomputing

Two categories of MD methods

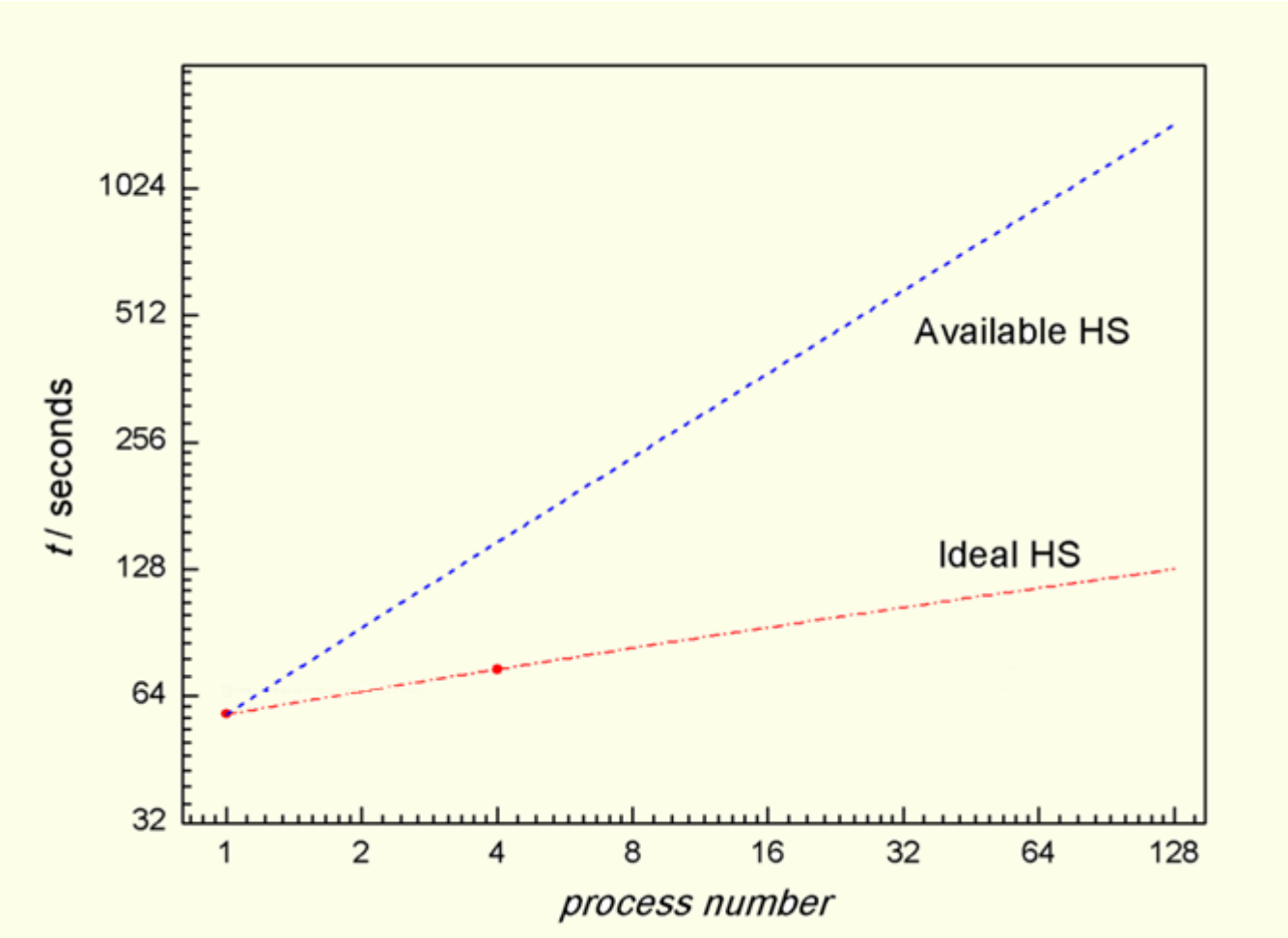
Model:	Soft Sphere (SS)	Hard Sphere (HS)
Algorithm	time-driven (synchronized)	event-driven (asynchronized)
Pros	scalable	accurate (machine err.) efficient (dilute)
Cons	inefficient (dilute) inaccurate (num. err.)	non-scalable ($N \log N \rightarrow \sqrt{N}$)

Hard sphere model and algorithm





Scalability of the event-driven algorithm



dash line: Available HS

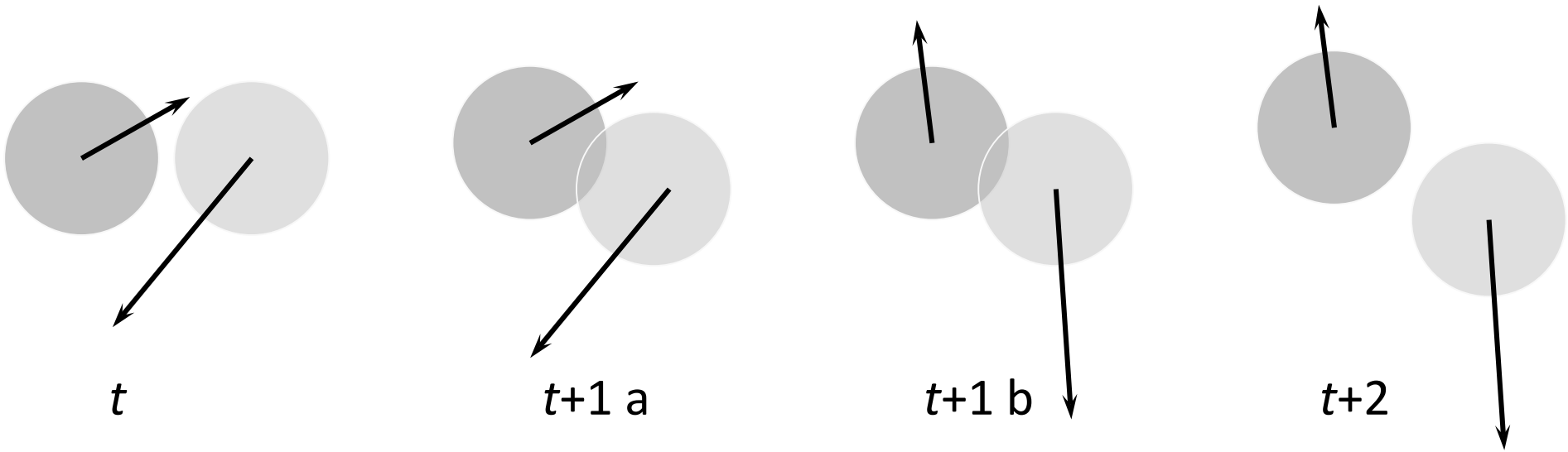
Miller et al., 2003. Computational Physics 193, 206-316

dash-dot line: Ideal HS parallelized perfectly

Zhang, Shen & Ge et al. 2016 *Molecular Simulation* 42: 1171-1182

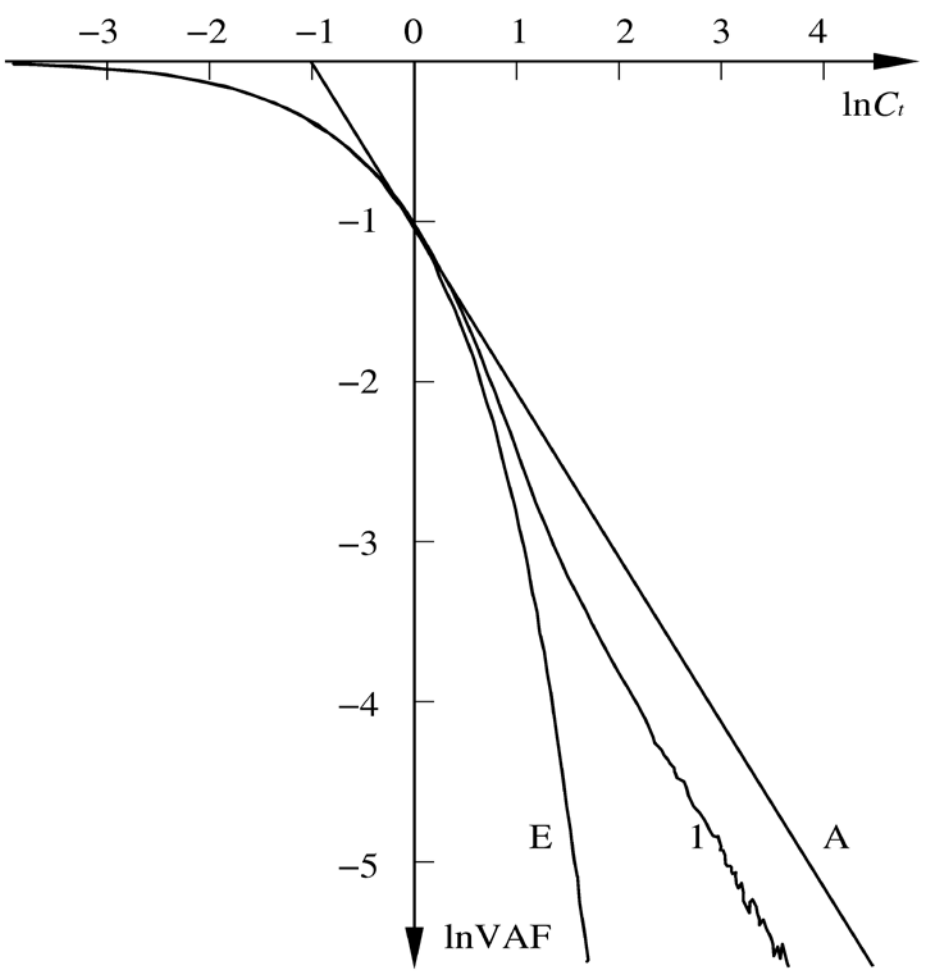
Pseudo-particle modeling for dilute gas: a combination of SS & HS

$$\mathbf{v}_1' = \mathbf{v}_1 + \frac{(1+e_{12})m_2}{m_1+m_2}\frac{(\mathbf{v}_1-\mathbf{v}_2)\cdot(\mathbf{P}_1-\mathbf{P}_2)}{(\mathbf{P}_2-\mathbf{P}_1)^2}(\mathbf{P}_2-\mathbf{P}_1)$$

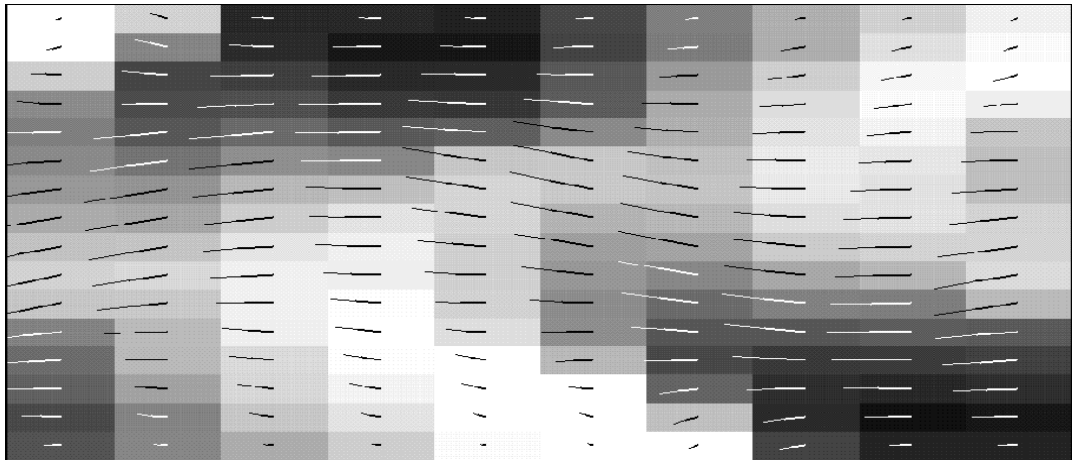


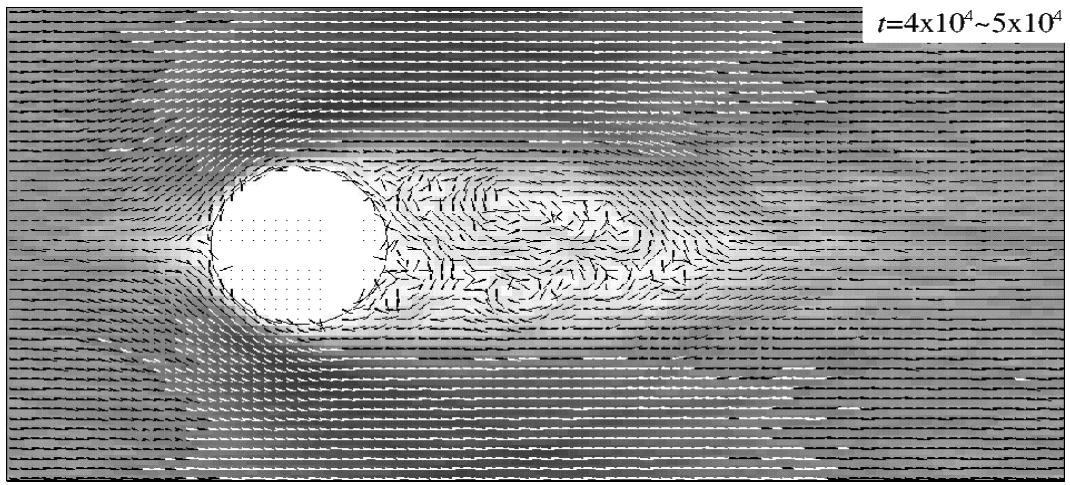
Ge & Li 2003 *Chem. Eng. Sci.* 58: 1565-1585; Chen & Ge 2010 *Particuology* 8:332-342

PPM for flow simulation



Long-time tail of
the velocity auto-correlation function (VAF)





TS waves in duct flow & Flow past a single cylinder

Properties of the pseudo-particles

Obtained in equilibrium molecular dynamics simulation

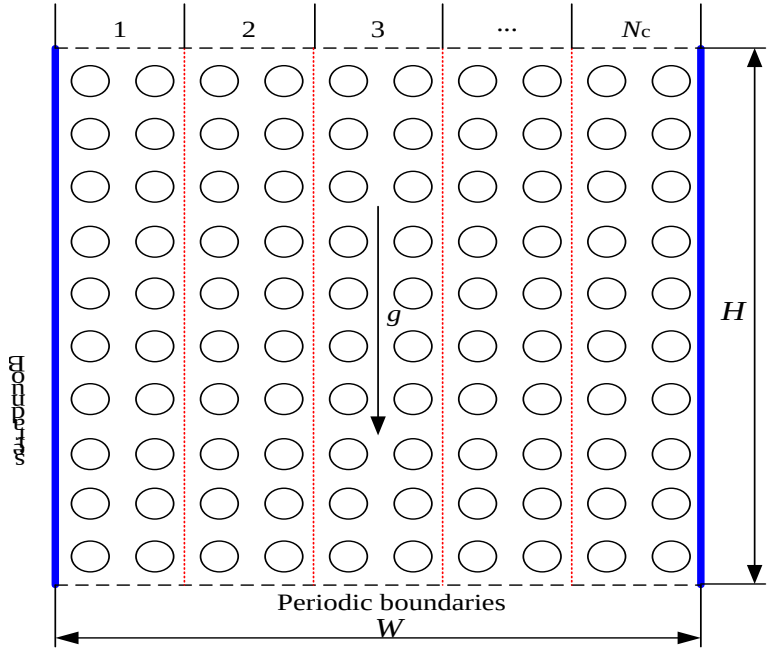
Mean free path $l = \sum_i s_i \Big/ n_{\text{colls}}$

Pressure $PV = Nk_{\text{B}}T + \frac{1}{dim}\frac{1}{t_{\text{obs}}}\sum_{\text{colls}} \mathbf{r}_{ij} \cdot \delta\mathbf{p}_i$

Self-diffusion coefficient $D = \frac{1}{2dim}\lim_{t\to\infty}\left\langle \left|\mathbf{r}_i(t) - \mathbf{r}_i(0)\right|^2 \right\rangle$

Obtained in non-equilibrium molecular dynamics simulation

Shearing viscosity $\nu = \frac{gW^2}{12U_{\text{m}}}$



Chen & Ge 2010 *Particuology* 8:332-342

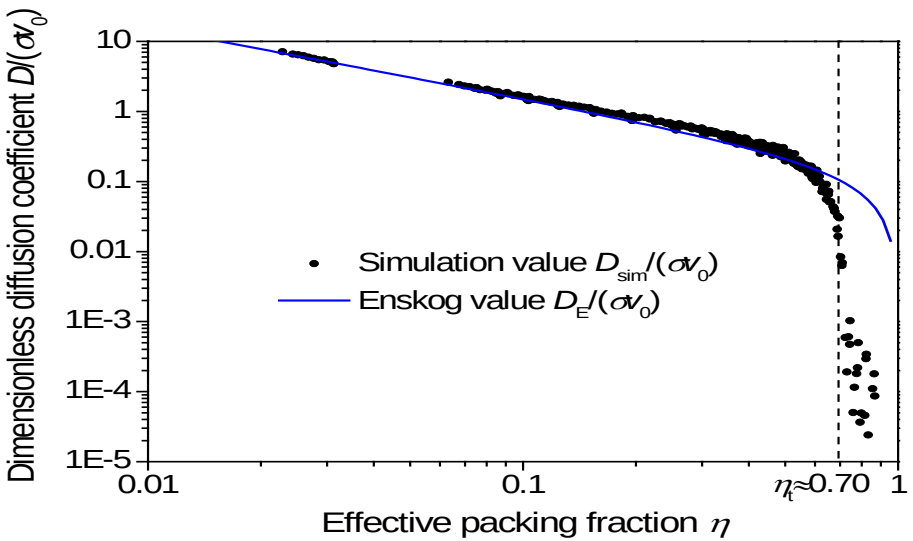
Effective self-diffusion coefficient

2D

Hard shere model

$$\chi = \frac{1-\eta/2}{(1-\eta)^2}$$

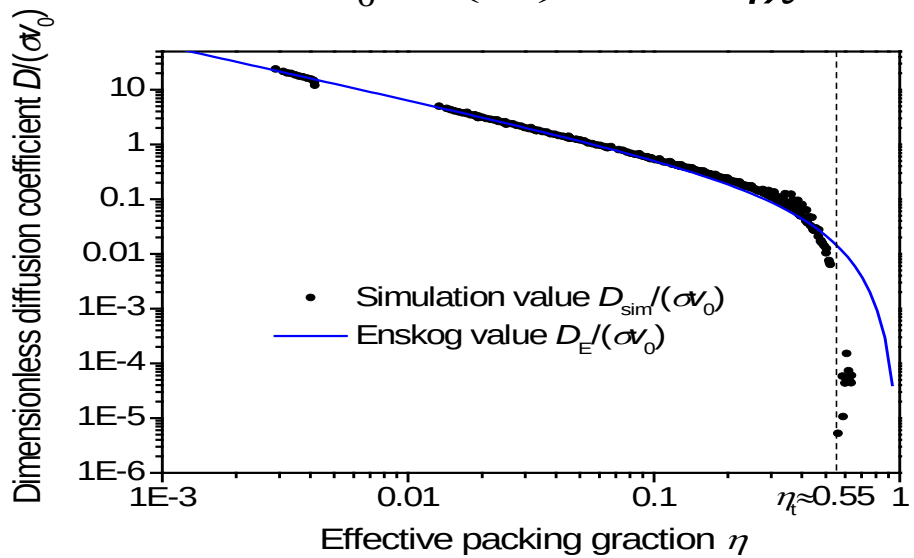
$$D_{\mathrm{E}}^{*} = \frac{D_{\mathrm{E}}}{\sigma v_0} = \left(\frac{\pi}{2}\right)^{1/2} \frac{1}{8\eta\chi}$$



3D

$$\chi = \frac{1-\eta/2}{(1-\eta)^3}$$

$$D_{\mathrm{E}}^{*} = \frac{D_{\mathrm{E}}}{\sigma v_0} = \left(\frac{\pi}{3}\right)^{1/2} \frac{1.01896}{16\eta\chi}$$



Effective shearing viscosity

2D

3D

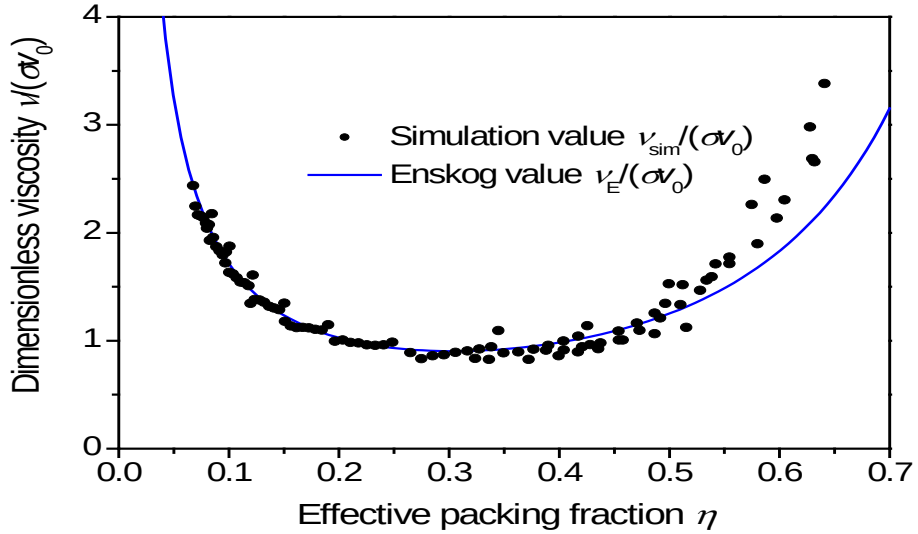
Hard sphere model

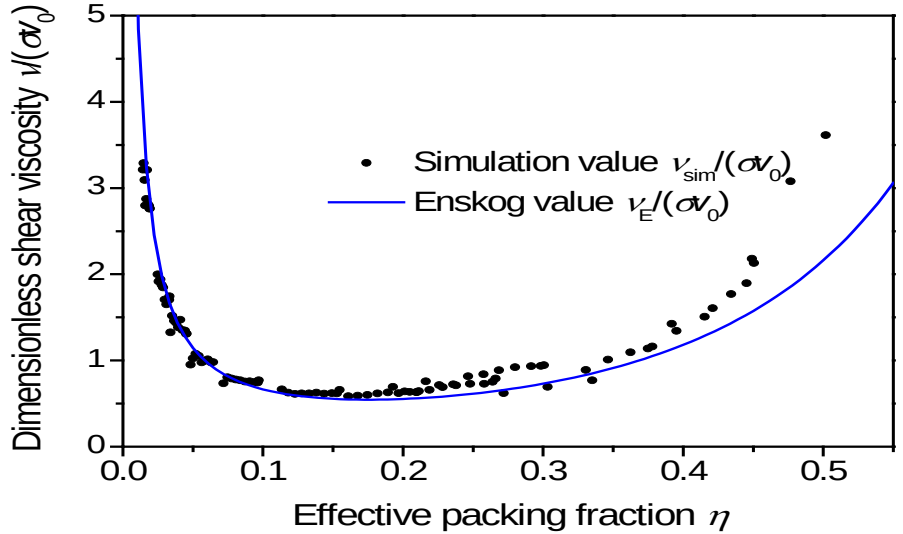
$$\chi = \frac{1-\eta/2}{(1-\eta)^2}$$

$$\chi = \frac{1-\eta/2}{(1-\eta)^3}$$

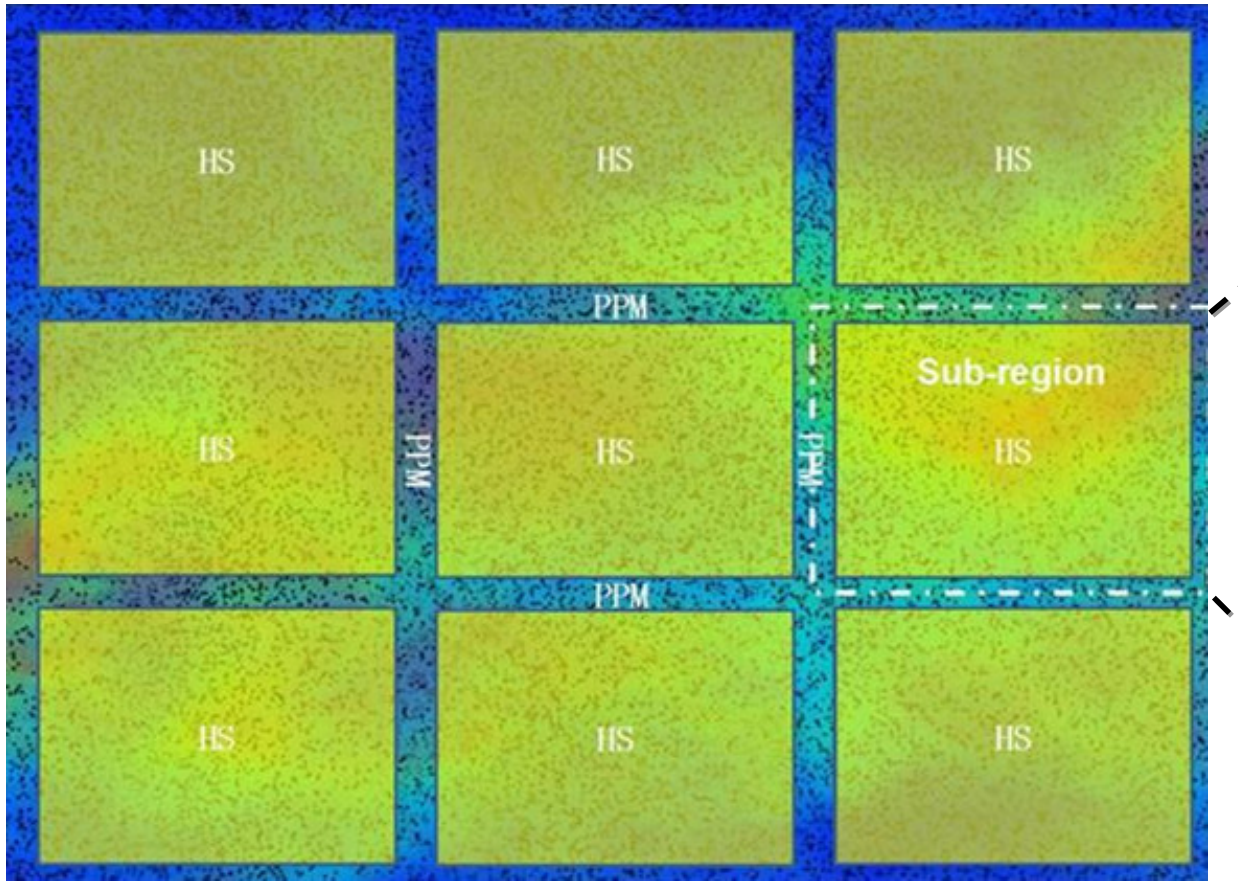
$$\nu_E^* = \frac{1}{8\eta}\left(\frac{\pi}{2}\right)^{1/2}\left[\frac{1}{\chi} + 2\eta + \left(1+\frac{8}{\pi}\right)\chi\eta^2\right]$$

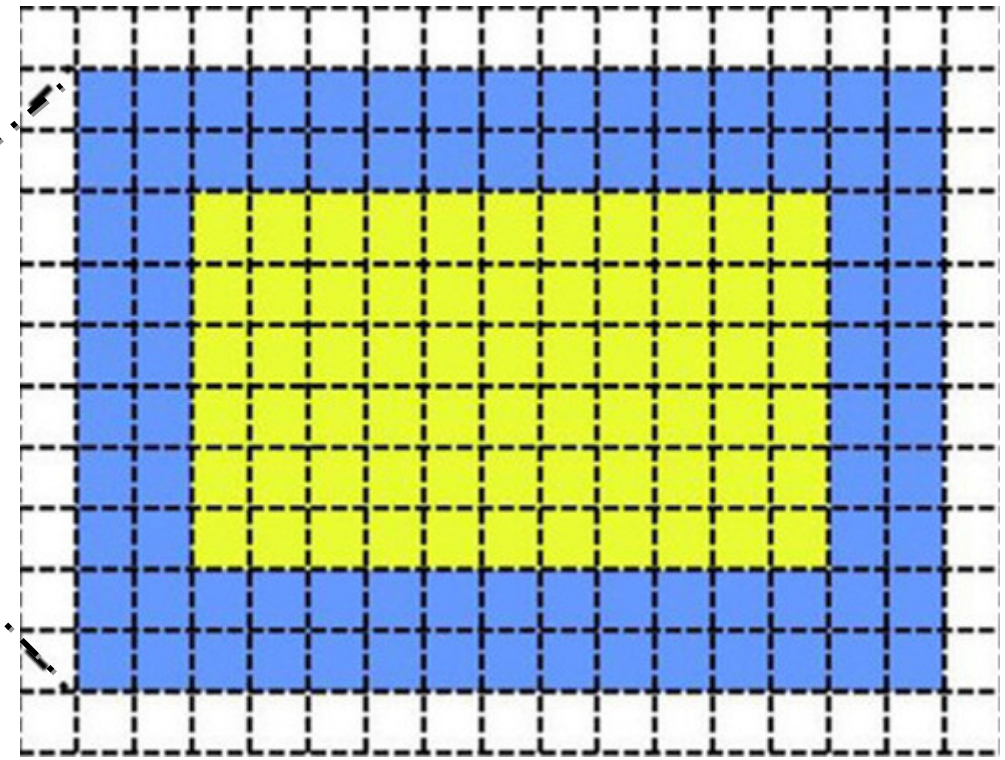
$$\nu_E^* = \frac{5}{96\chi\eta}\left(\frac{\pi}{3}\right)^{1/2}\left[\left(1+\frac{8}{5}\chi\eta\right)^2 + \frac{768}{25\pi}(\chi\eta)^2\right]$$





Simulation of dilute gas: Hard sphere + pseudo-particle modeling

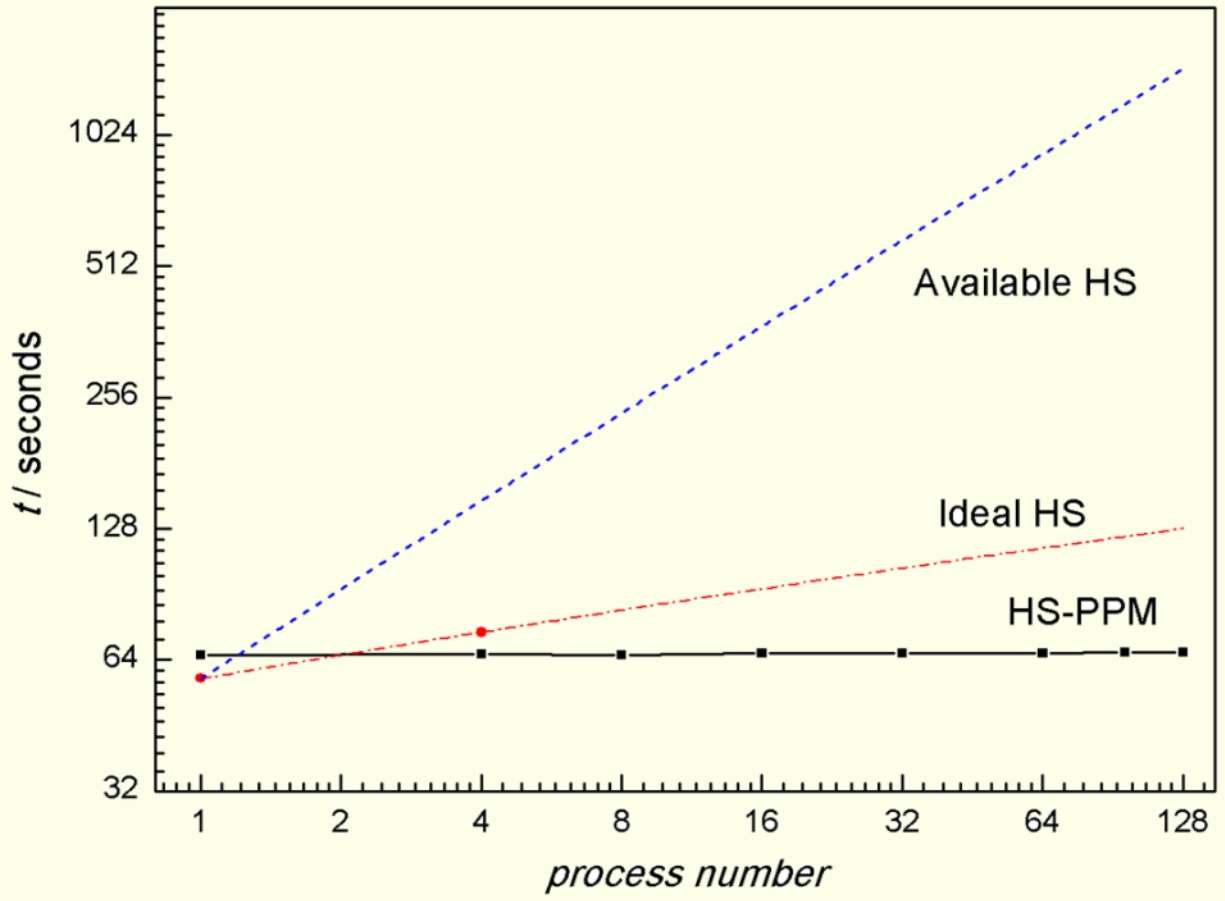




PPM HS Buffer

Zhang, Shen & Ge et al. 2016 *Molecular Simulation* 42: 1171-1182

Demonstration of scalability



dash line: Available HS

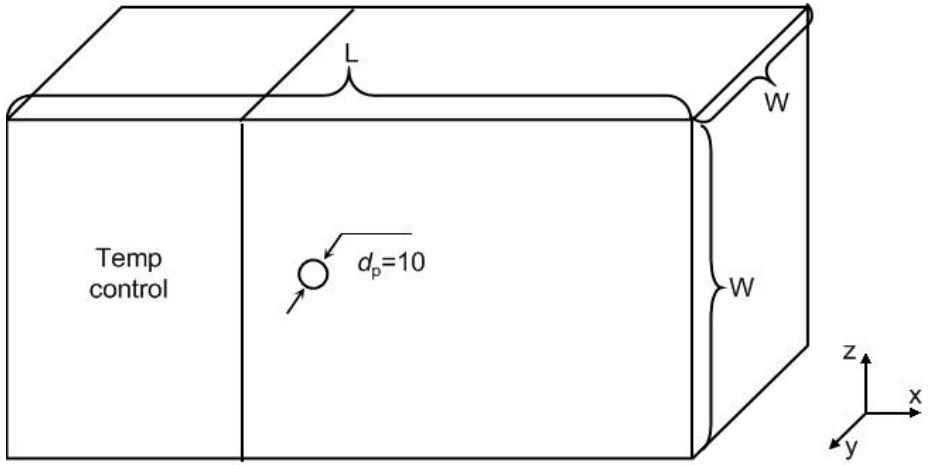
Miller et al., 2003. Computational Physics 193, 206-316

dash-dot line: Ideal HS parallelized perfectly

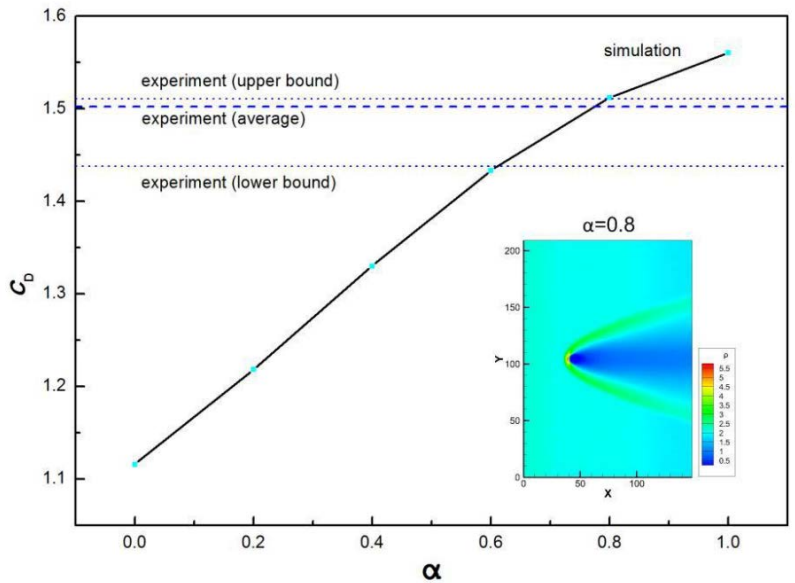
dash-dot line: HS-PPM multiple processes with same scale on each process

Zhang, Shen & Ge et al. 2016 *Molecular Simulation* 42: 1171-1182

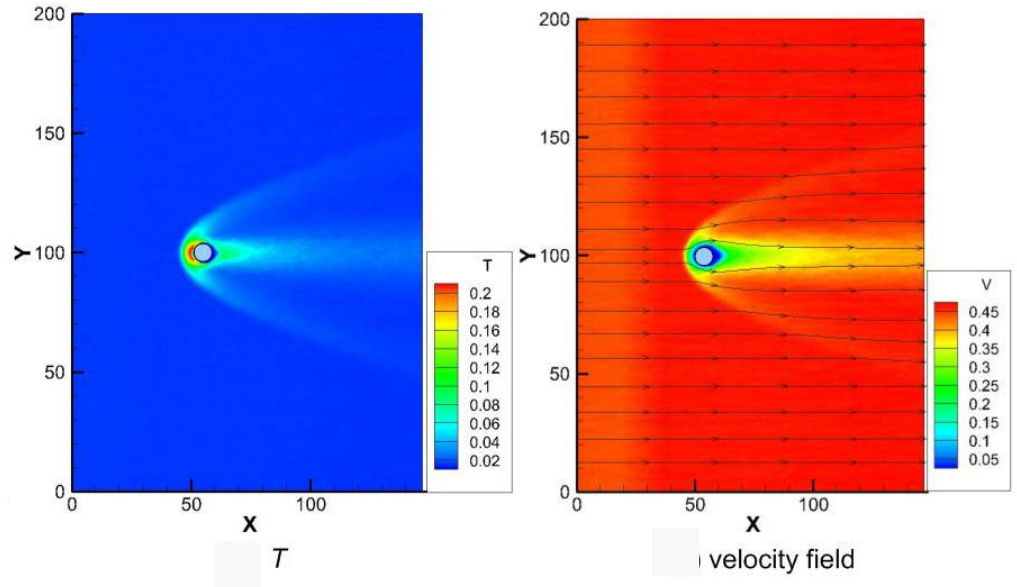
Simulation of flow past a single sphere



Ma=3.865
Re=104

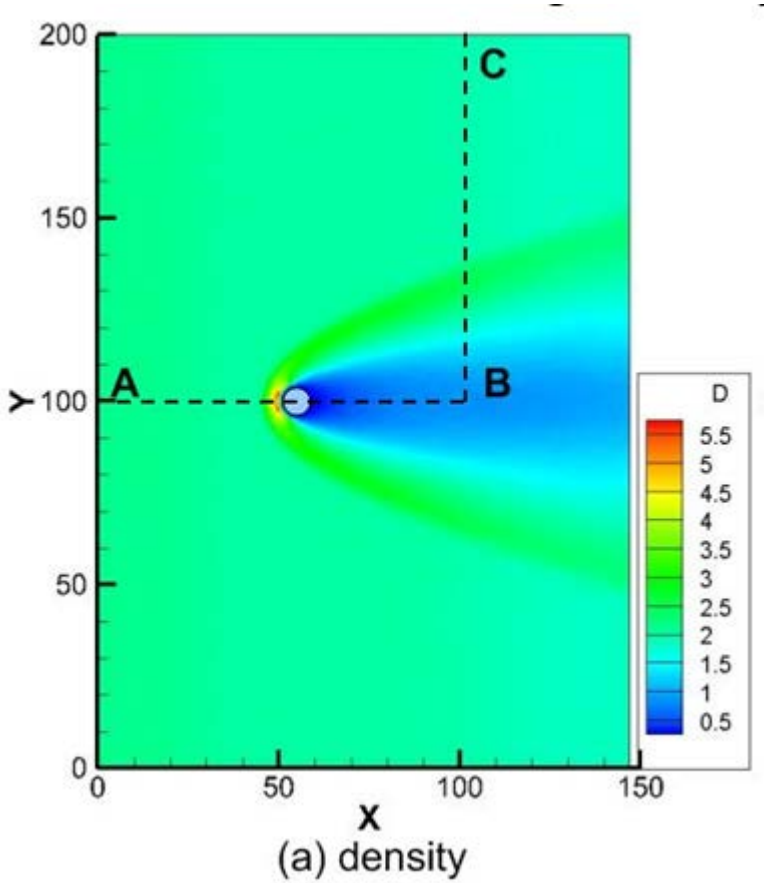


Comparison of the drag coefficients from simulation with experiments

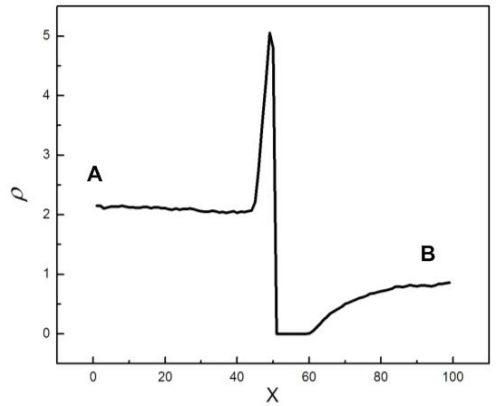


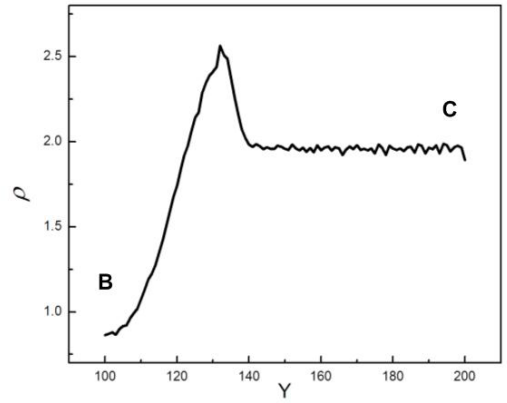
Flow field across the shockwave

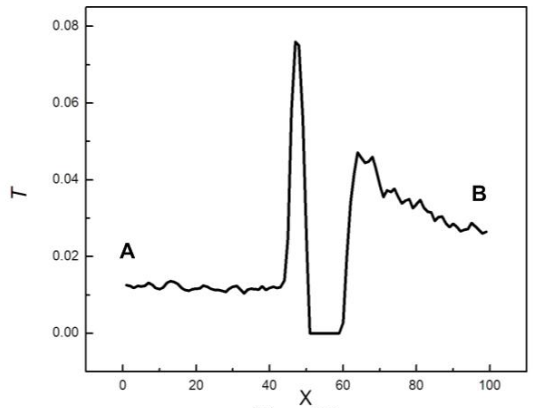
Simulation of flow past a single sphere



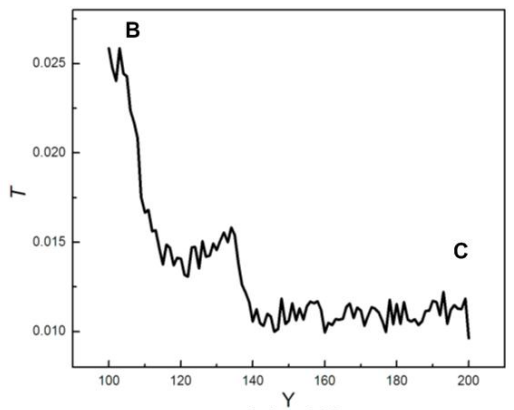
(a) density







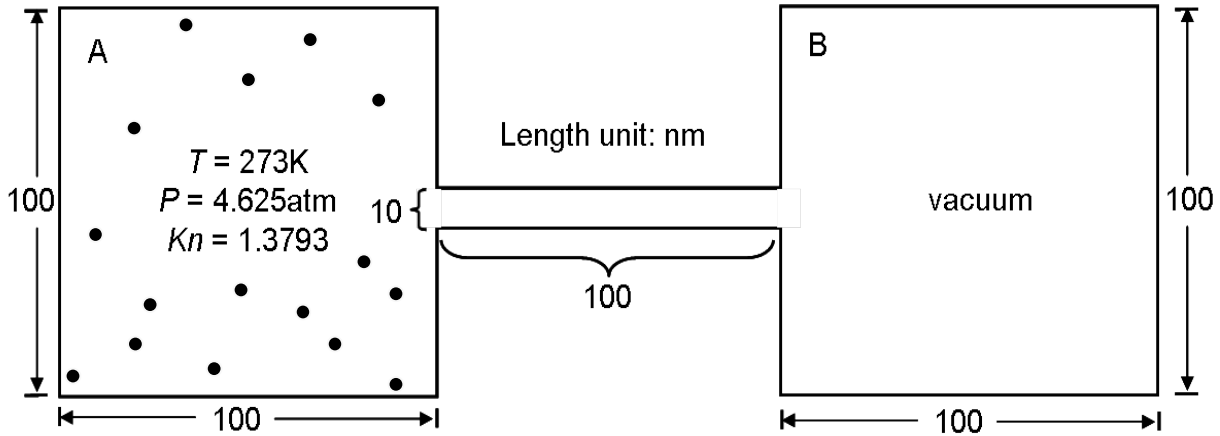
(d) y=100

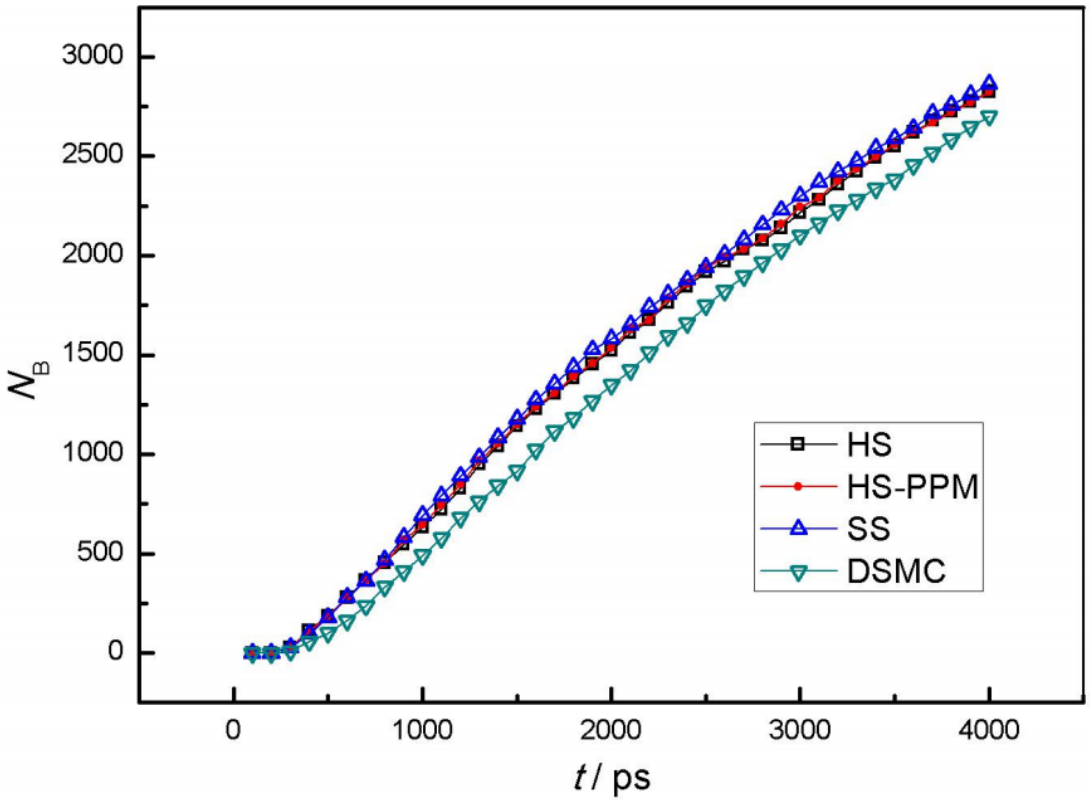


(e) x=100

Flow distribution at two planes across the shockwave

The diffusion between two chambers





The number of particles (NB) in chamber B during the diffusion process

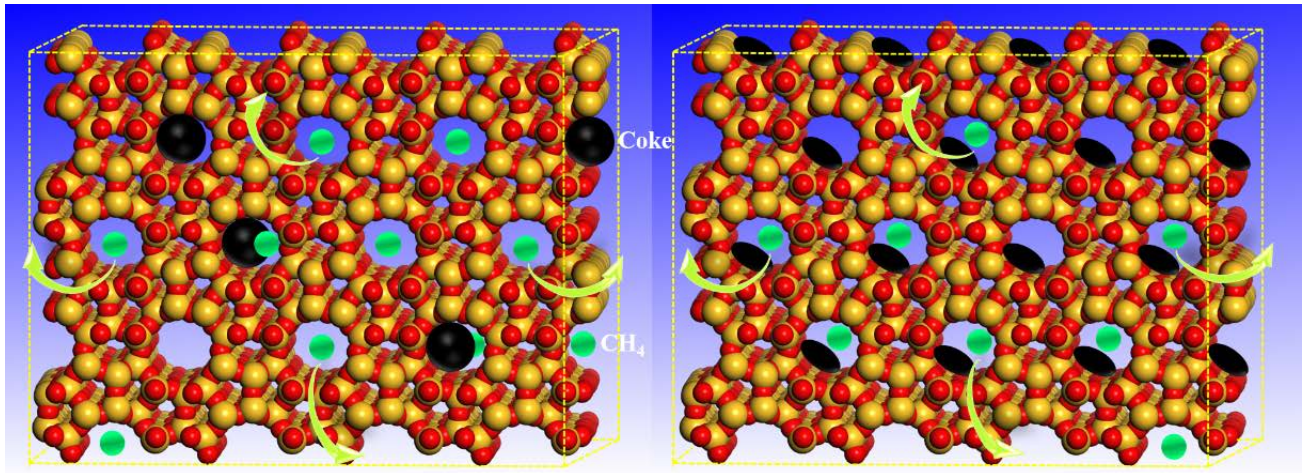
Zhang, Shen & Ge et al. 2016 Molecular Simulation 42: 1171-1182;

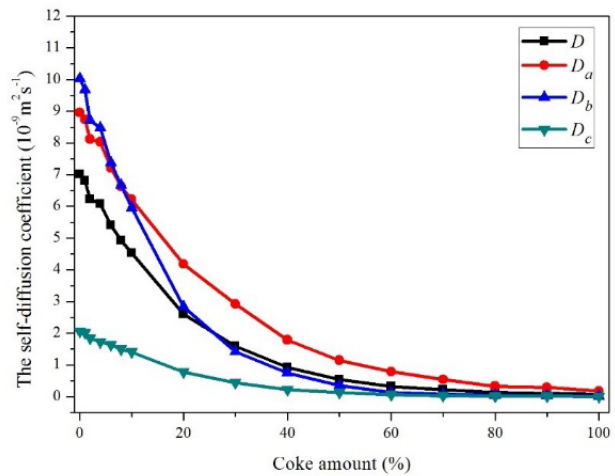
Zhang et al. 2016. *Comp. & Appl. Chem.* 33(11):1135-1144 (In Chinese)

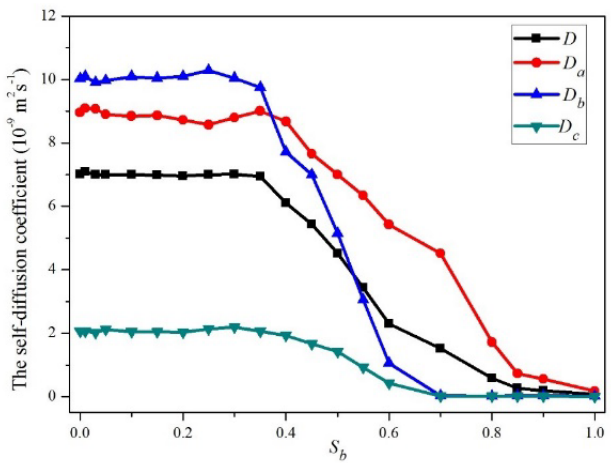
Effect of coke on gas diffusion in zeolites

Coke Model I

Coke Model II





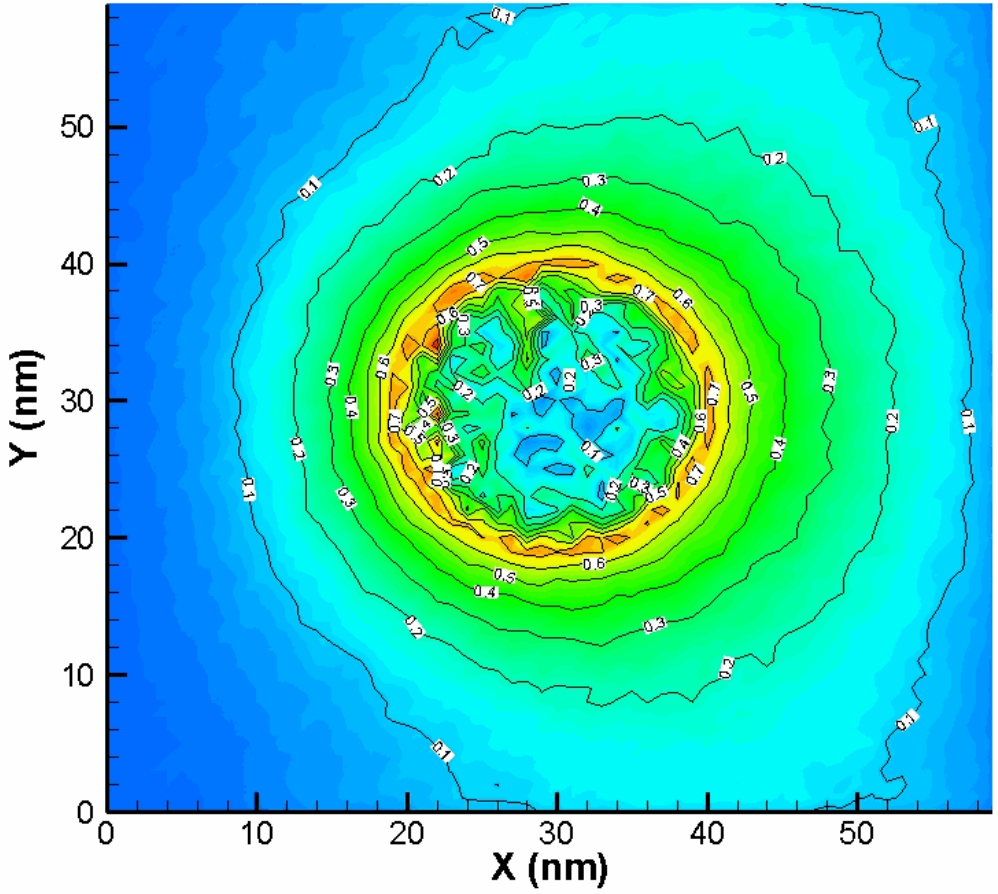


ZSM-5 zeolite (MFI) : 8×8×8 (u.c)
Gas properties similar to methane at 723K & 1tam
Gas loading: 4 molecules/u.c.
Coke deposition at T12 sites.

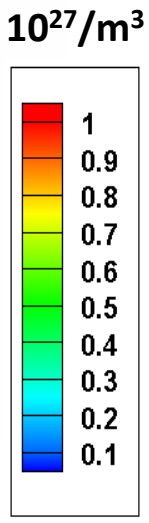
Li, Zhang, Li, Liu & Ge,
Chemical Engineering Journal,
2017, 320: 458-467

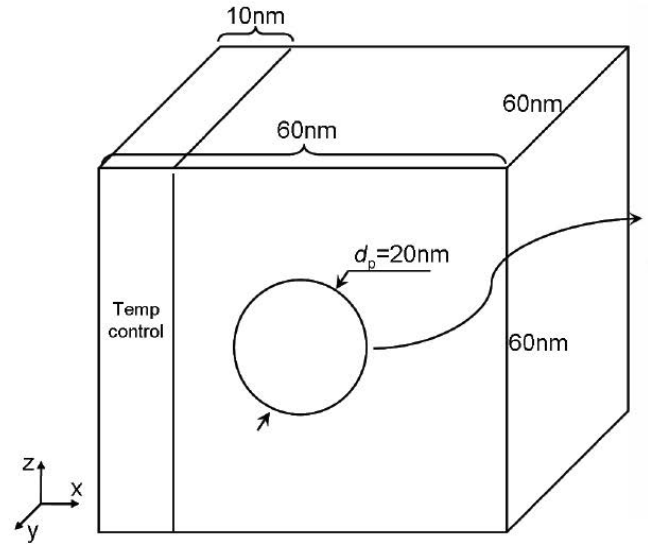
Self-diffusion coefficients vs. coke amount for the two coke formation mechanisms

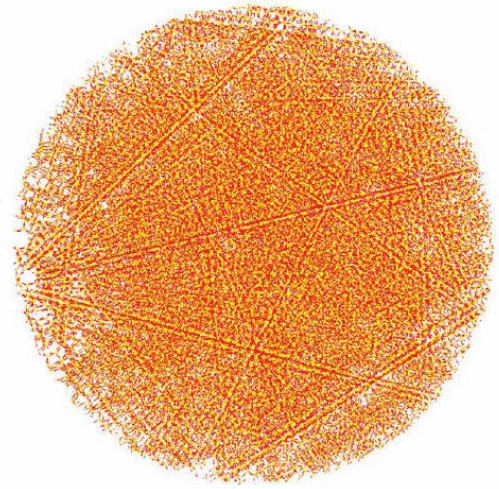
Flow-diffusion-reaction in a porous particle



The number density distribution of products







Solid material structure
similar to ZSM-5

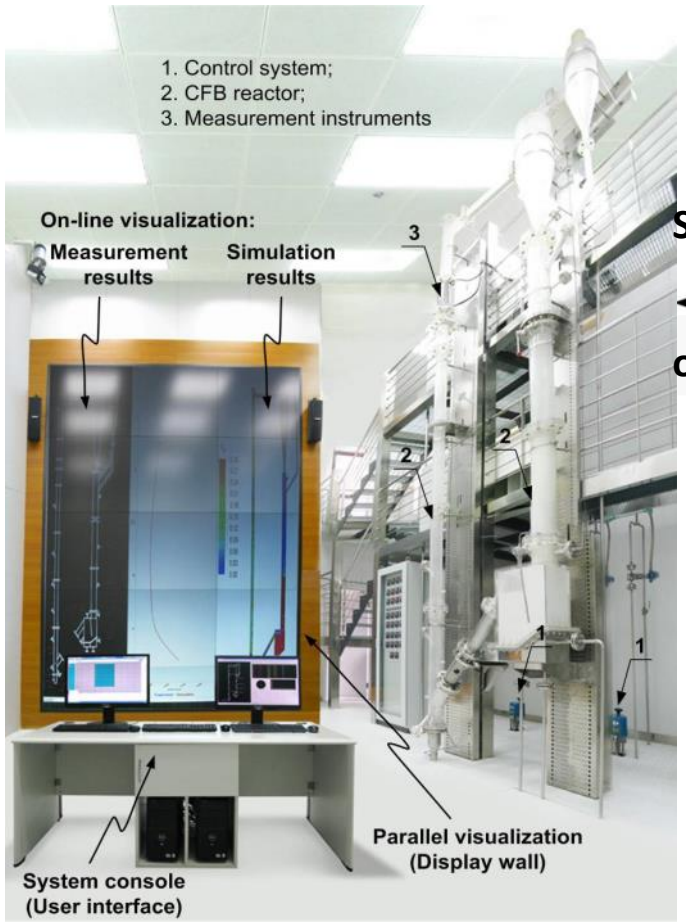
Gas properties
similar to methane
at 723K & 1tam

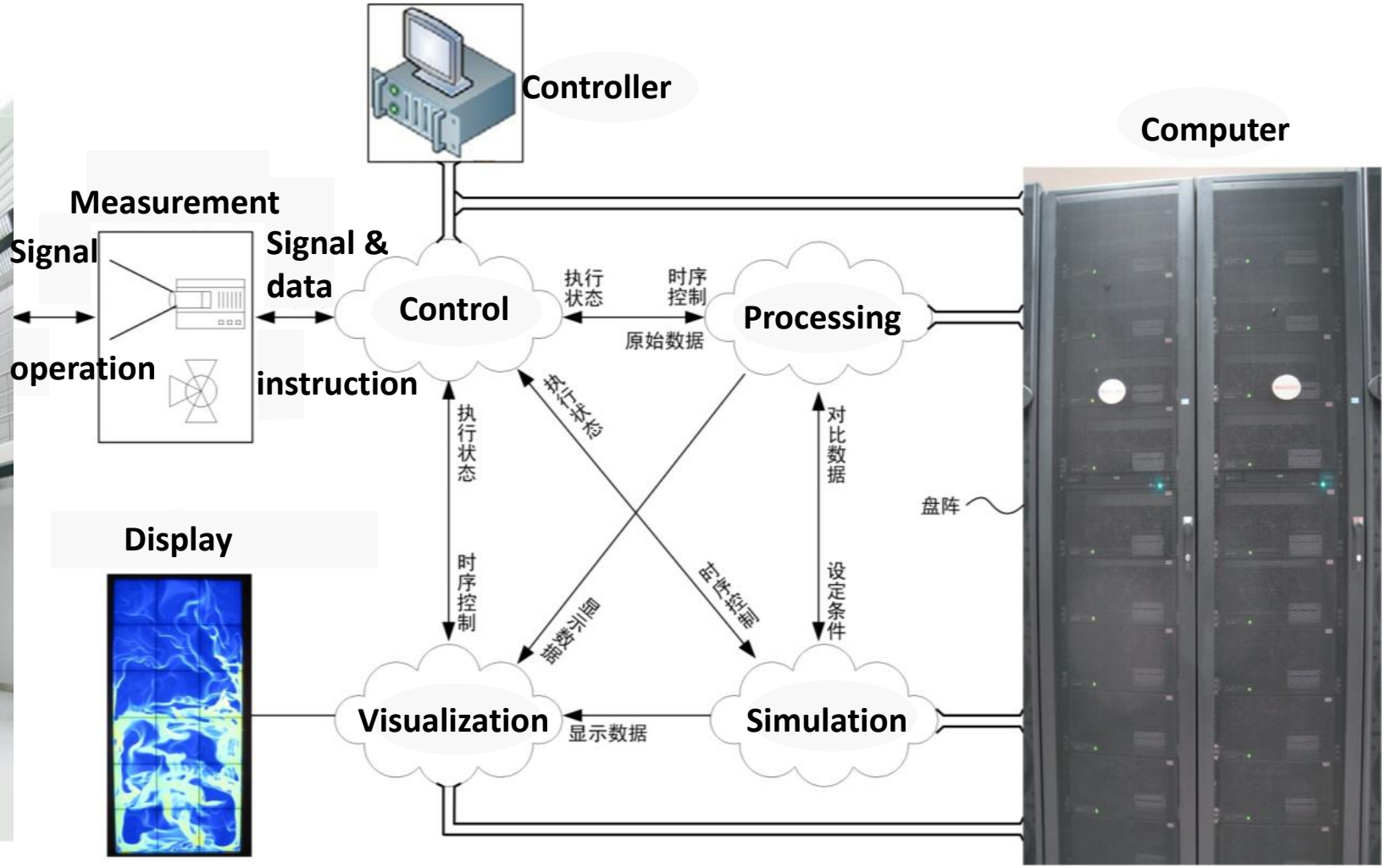
Zhang et al. 2016 *IPE Internal Report*

Virtual Process Engineering

from reactions to reactors

The VPE platform at CAS-IPE



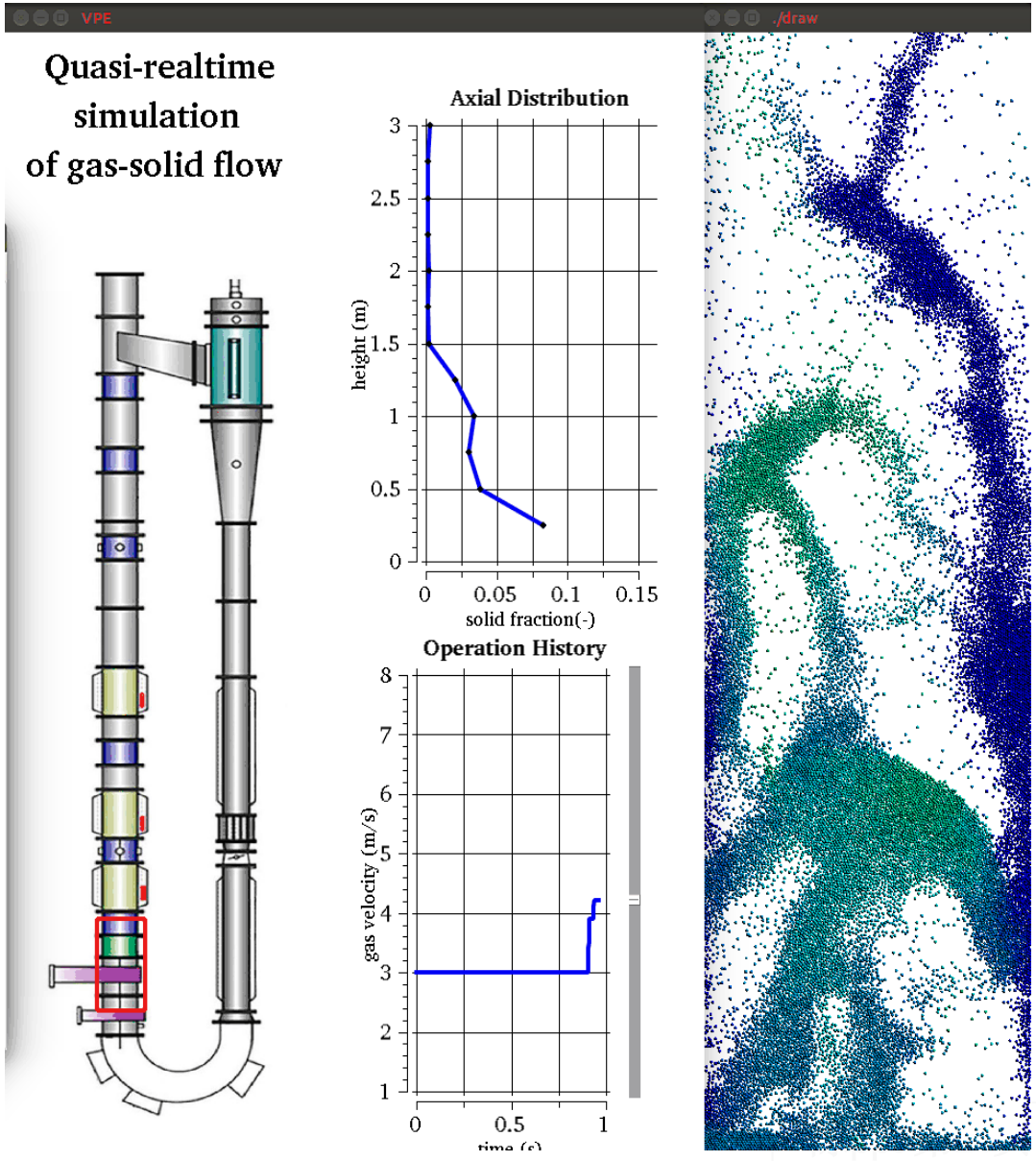


Experiment - Measurement - Computation - Visualization - Control integrated

Ge et al. 2011 *Chem. Eng. Sci.* 66:4426-4458; Liu et al. 2012 *Chem. Eng. Proc.* 108:28-33

Offline → Online interactive simulation

real solids: ~ 10 billion
CG solids: ~ 0.3 million
d_p: 200 microns
~ 1/30-1/50 realtime speed
@ 0.1ms time step



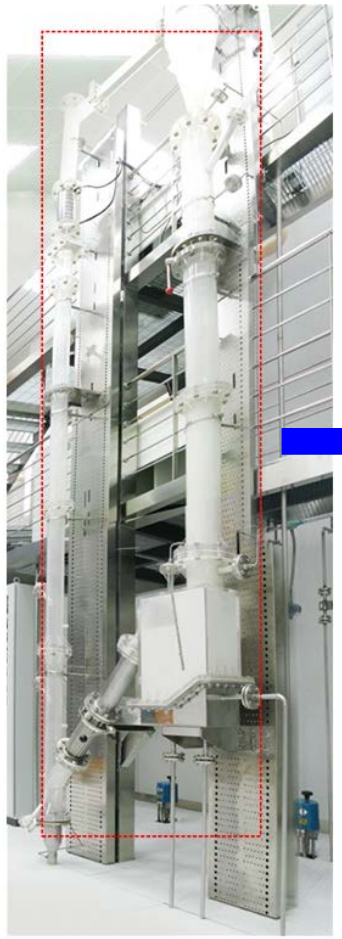
Ge et al. 2015 *Chem. Eng. & Tech.* 38:575-584;

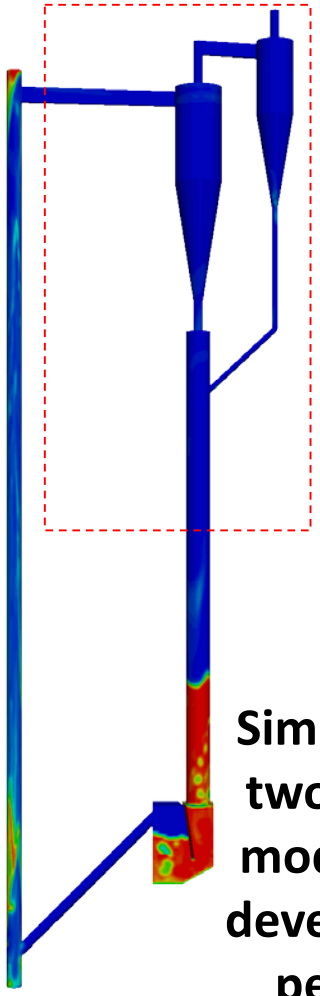
Lu et al. 2016 *Chem. Eng. Sci.* 155:314-337

Xu et al. 2017 *Internal Report*

Discrete simulation of a CFB at lab-scale

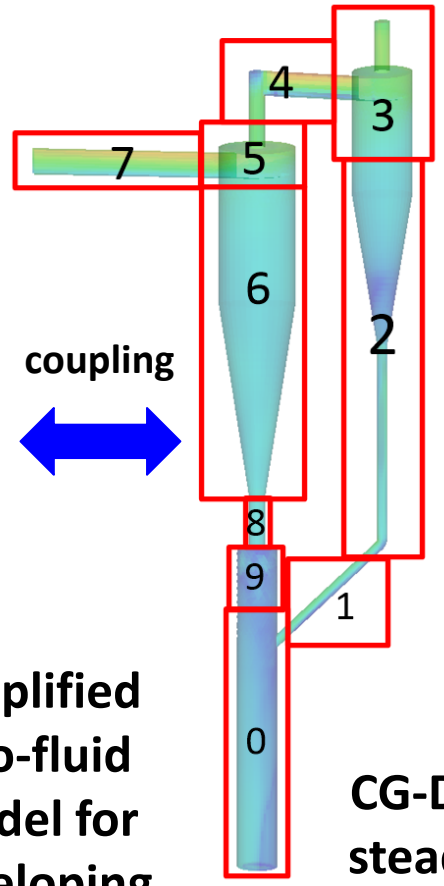
Physical system





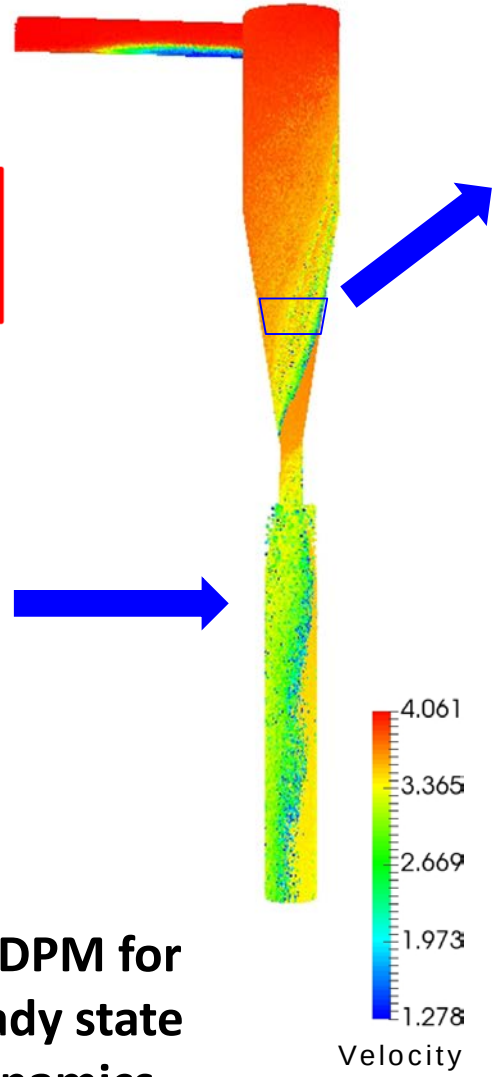
Simplified two-fluid model for developing period

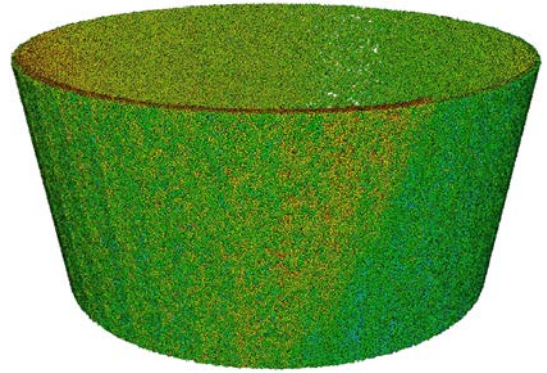
decomposition scheme



coupling

CG-DPM for steady state dynamics

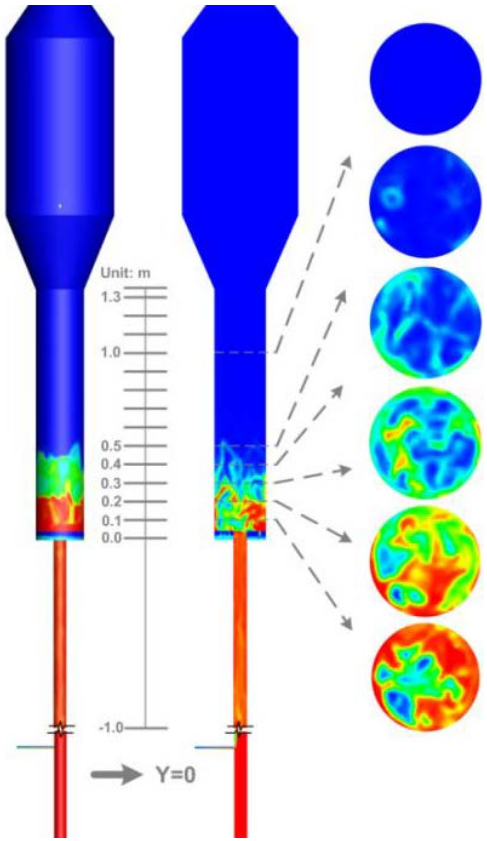


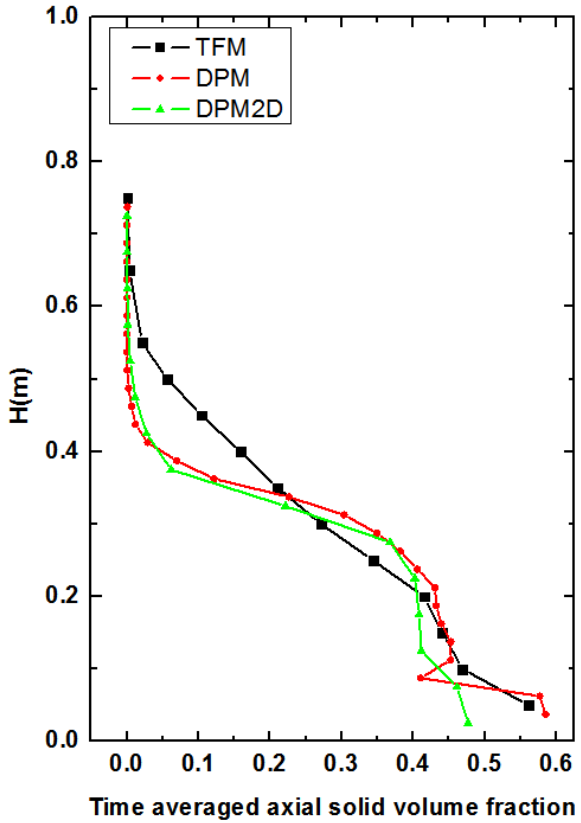


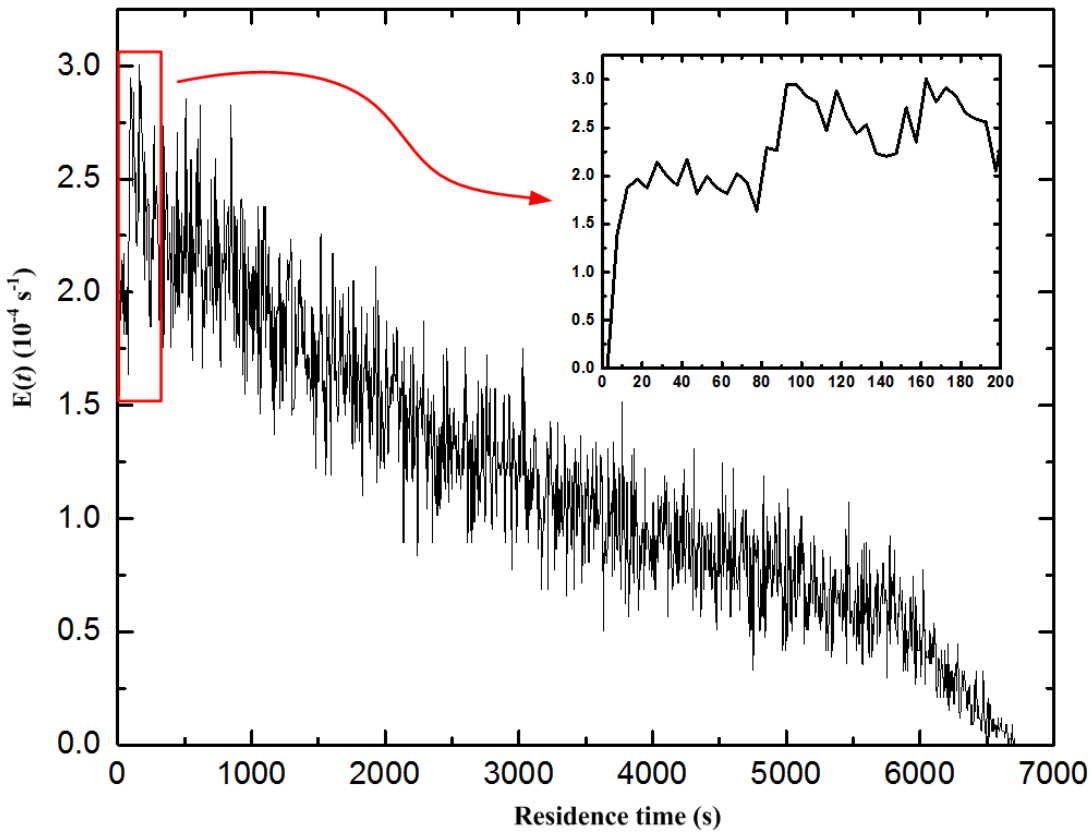
CG_{ratio}	3
Particle size distribution	10^{-4}m (1.23 1.85 2.46) %mass (5 90 5)
$N_{particle}$	**81.5 Million**
N_{cell}	94,694
K80	**54**
CPU	108 cores
dt_{solid}	2.0e-6
dt_{gas}	4.0e-5
Speed	**≈40s/day**

Xu et al. 2017 *Internal Report*

Very long time simulation at industrial scale





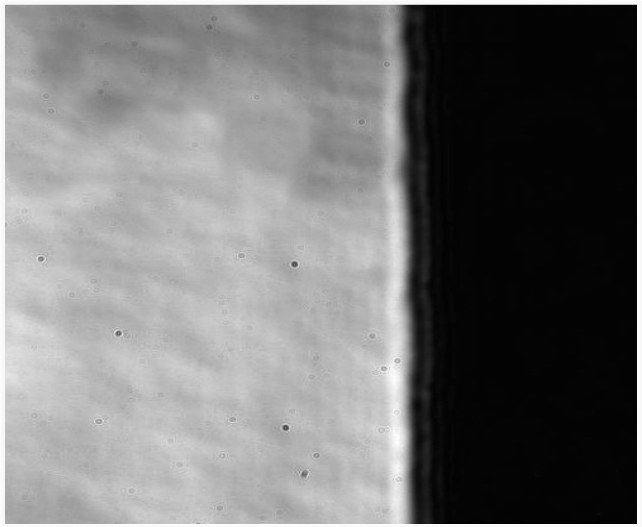


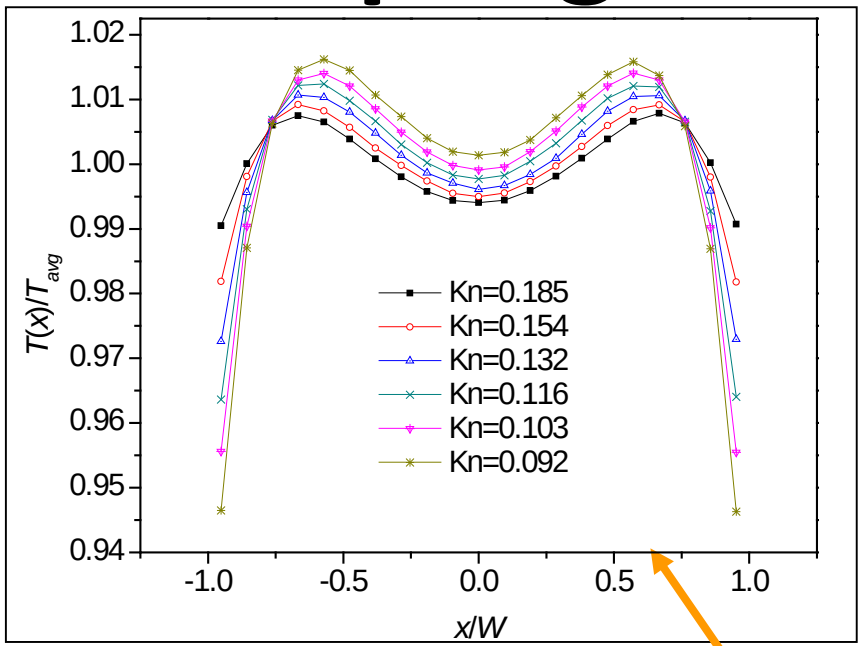
22x(CPU+GPU), 640s/day, 6800s totally

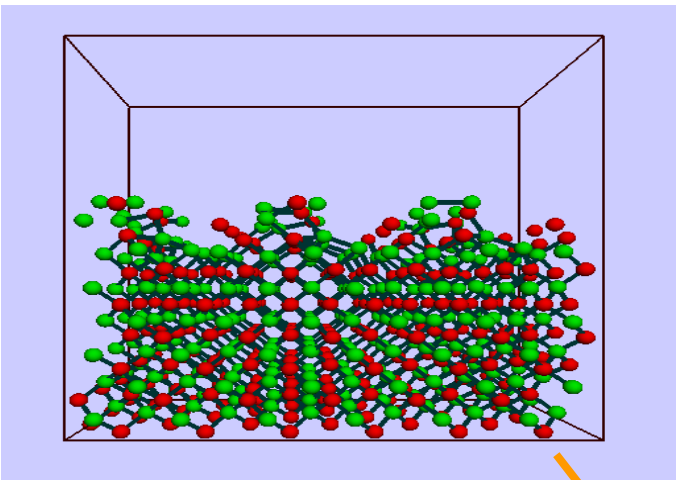
Lu et al. 2016 *Chem. Eng. Sci.* in revision; TFM data from Lu et al. 2015 *Internal Report*

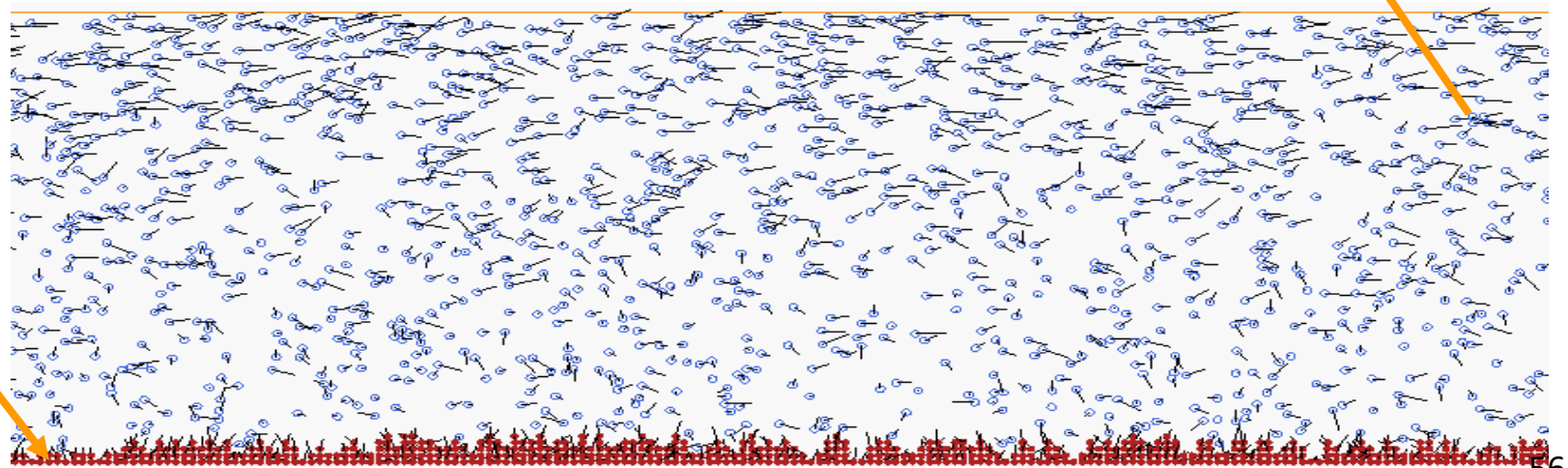
Reaction-diffusion-flow coupling

Xu et al. 2015 *Chem. Eng. Sci.* 121:200-216



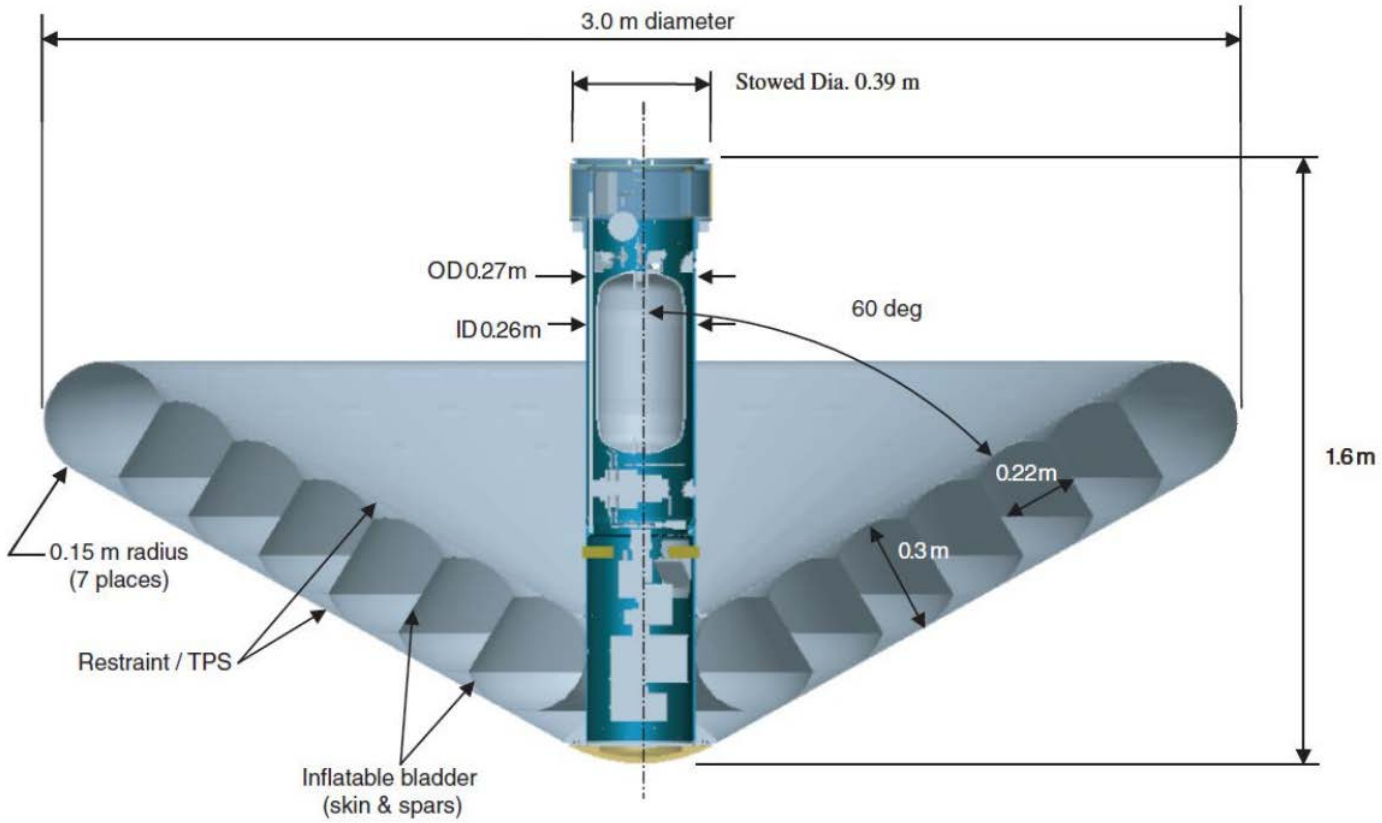






Shen & Ge, Phys. Rev. E, 2010

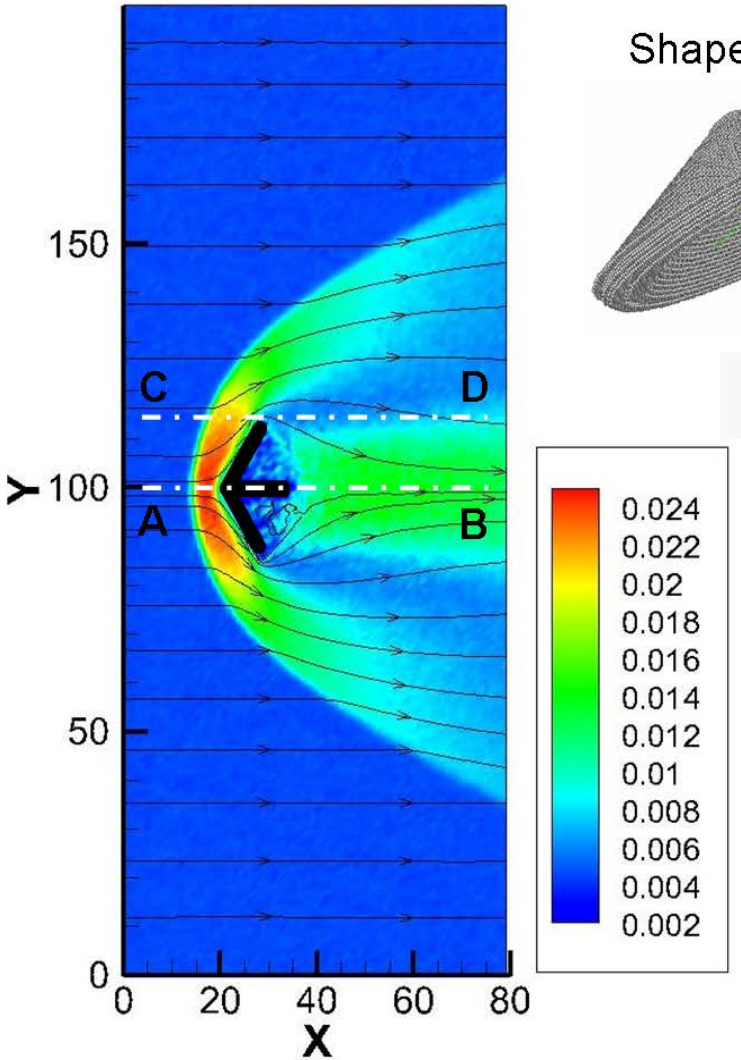
Inflatable reentry vehicle experiment (IRVE)



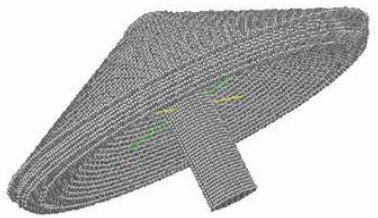
Case	Ma	Kn	d_{HS}	d_{PP}	T	v_t	v_m	η
IRVE	3.99	0.0168	0.0600	0.0632	188	0.0675	0.201	3.5×10^{-3}

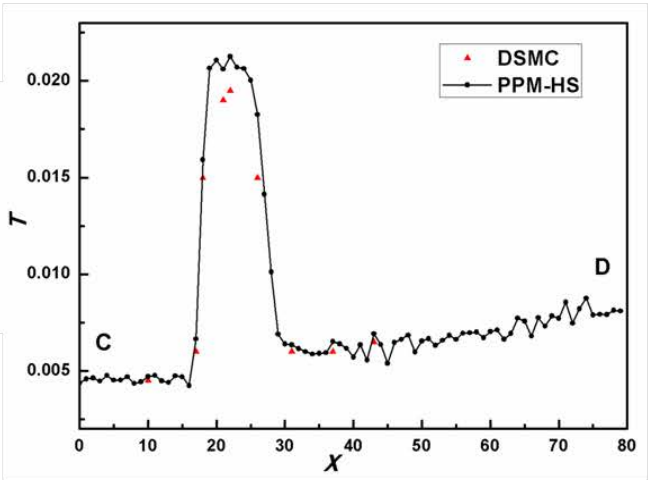
Simulations on IRVE

The flow field and temperature distribution of the simulation of IRVE

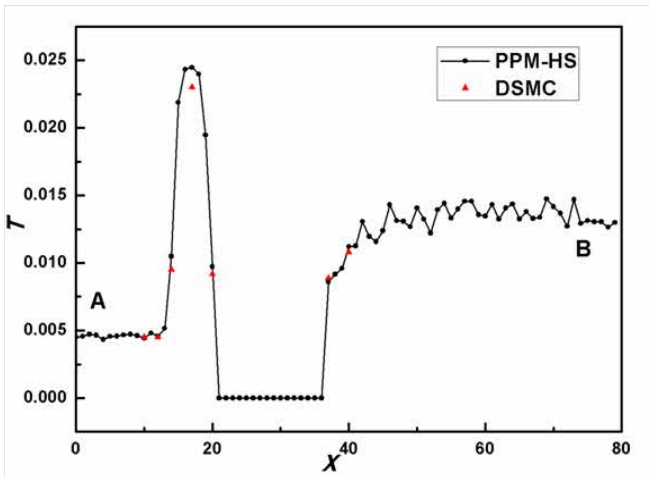


Shape of IRVE





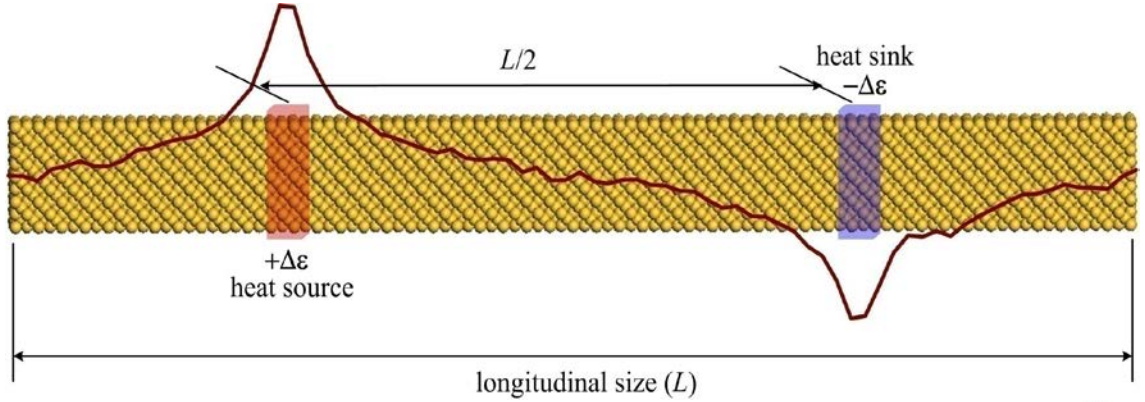
The simulation shape of IRVE



The temperature profiles of two crossing lines

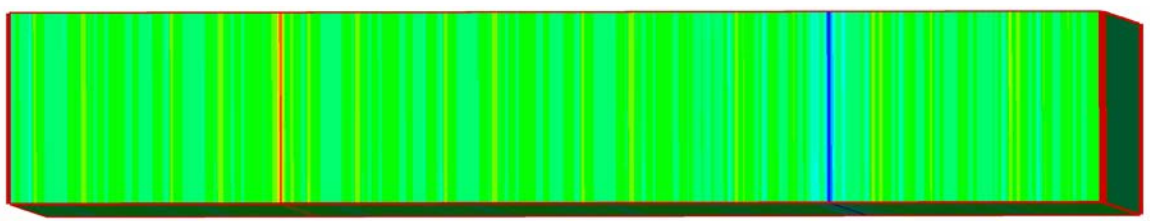
Zhang et al. 2016. *Comp. & Appl. Chem.* 33(11):1135-1144 (In Chinese)

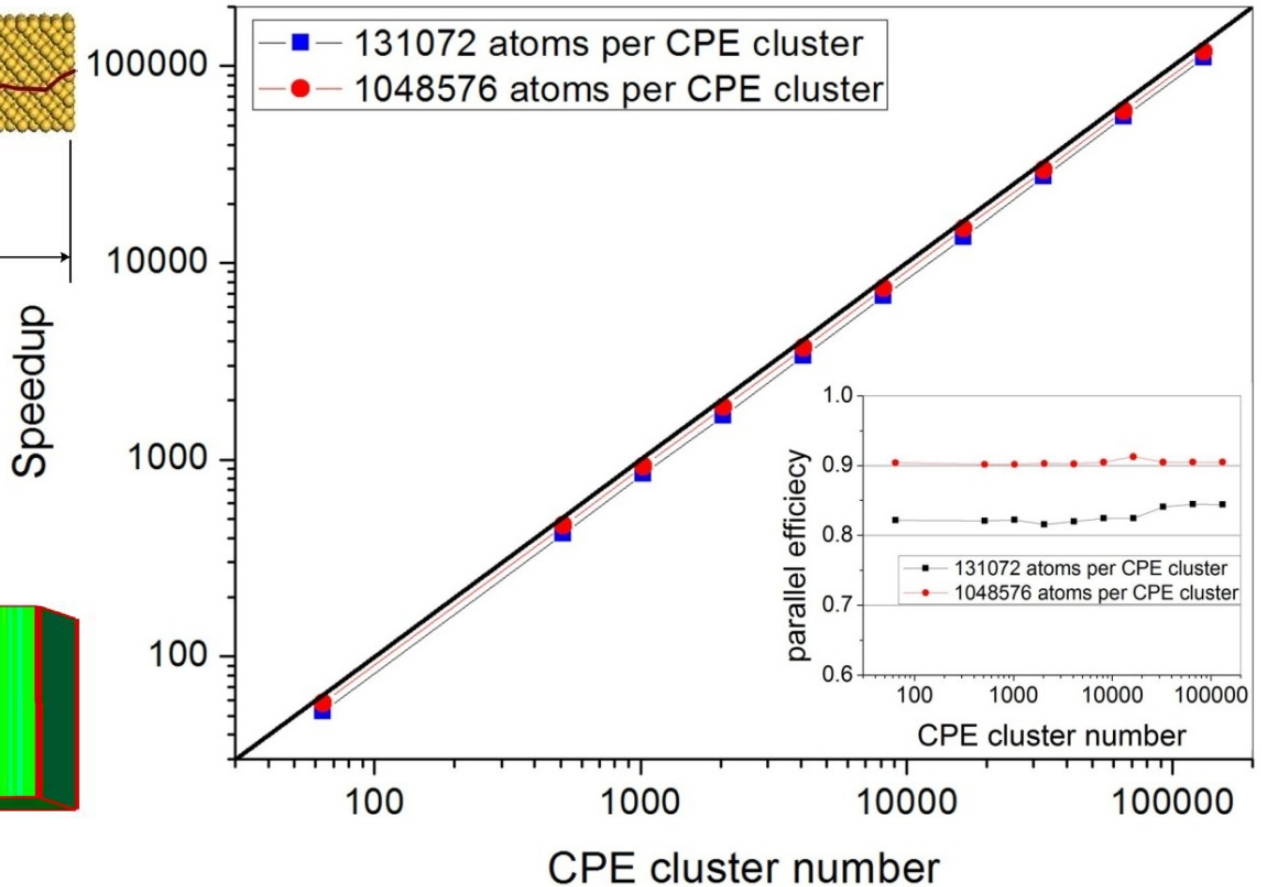
Full system test on *Haihu Light* (125PF)



Fu et al. 2016 *Sci. China: Info. Sci.* 59(7):072001

The Sunway TaihuLight supercomputer system and applications.





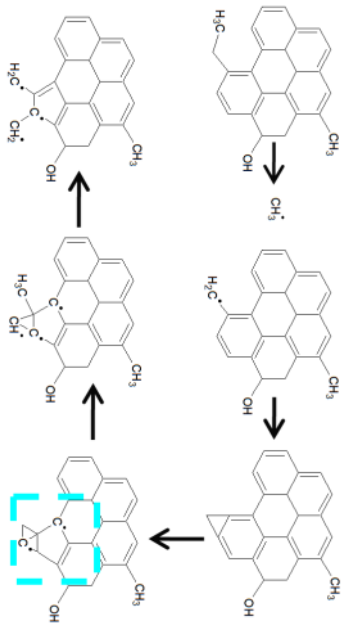
dp>60 nm, length>55mm

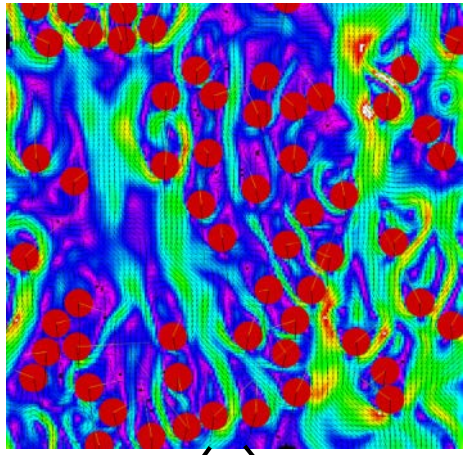
10.27 million cores (160K CPEs), 8.5-17.6Pflops sustainable performance

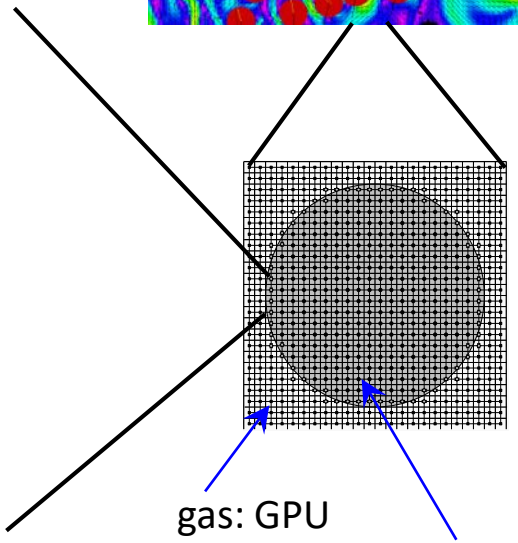
from Reactions to Reactors

Rcp= ratio of computing time to real time

Rcp~10^12







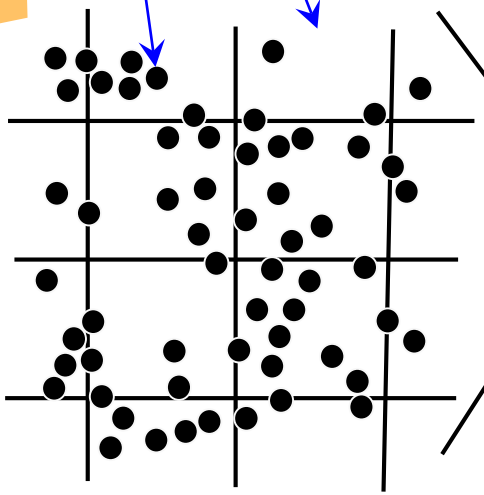
gas: GPU

solid particle: CPU

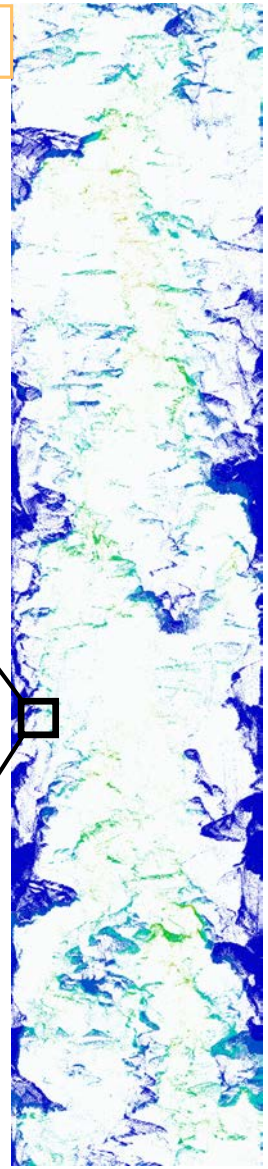
Rcp~2000

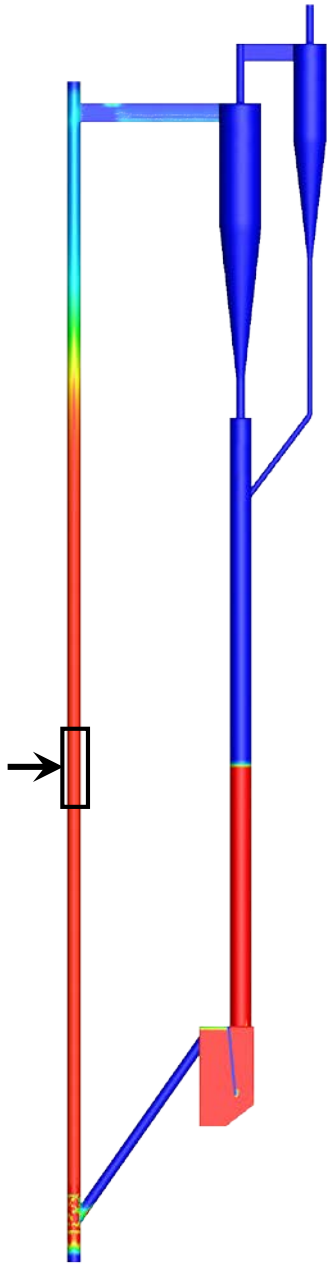
solid particle (silicon powder): GPU

gas (silane): CPU



Rcp~50





molecular scale → particle scale → reactor scale

Acknowledgements:

NSFC MOF MOST CAS

SinoPec PetroChina BaoSteel YeTech SynFuels

Alstom BASF BHPb BP EDF GE

Intel nVidia Shell Total Unilever

Thank you!

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